Robust Summaries
ACC FND Amides Category I - FND Amides
September 16, 2004

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2.1 MELTING POINT

Test Substance

Identity:	Stearamide (CAS RN 124-26-5)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	Standard reference book information; no experimental details provided.

Results

Melting point:	109 °C
Decomposition:	Not determined
Sublimation:	Not determined
Remarks:	

Conclusions

Remarks:	The melting point was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; secondary literature source.

References

Weast, R. C., (ed). 1979. CRC Handbook of Chemistry and Physics, 60th Edition. CRC Press, Boca Raton, FL, U. S.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	51
Remarks:	

2.1 MELTING POINT

Test Substance

Identity:	Oleamide (CAS RN 301-02-0)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	Standard reference book information; no experimental details provided.

Results

Melting point:	76 °C
Decomposition:	Not determined
Sublimation:	Not determined
Remarks:	

Conclusions

Remarks:	The melting point was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; secondary literature source.

References

Weast, R. C. and M. J. Astle, (eds). 1980. CRC Handbook of Chemistry and Physics, 60th Edition. CRC Press, Boca Raton, FL, U. S.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	74
Remarks:	

2.1 MELTING POINT

Test Substance

Identity:	13-Docosenamide, (Z)- (CAS RN 112-84-5; Erucamide)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Program (v 1.41) – The weighted mean was calculated using the values derived from the Joback Group Contribution Method and Gold and Ogle Method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Melting Point:	Estimated (weighted mean) = 183 °C Experimental database match = 77.5 °C
Decomposition:	Not applicable
Sublimation:	Not applicable
Remarks:	Following are the results from the model output (melting point only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:
  Name     :  13-DECOSENAMIDE (CIS)
  CAS Num  :  000112-84-5
  Exp MP (deg C):  77.5

SMILES : O=C(N)CCCCCCCCCCCC=CCCCCCCCC
CHEM   : 13-Docosenamide, (Z)-
MOL FOR: C22 H43 N1 O1
MOL WT : 337.59
---------------------- SUMMARY MPBPWIN v1.41 -----------------
Melting Point:  294.56 deg C (Adapted Joback Method)
Melting Point:  155.54 deg C (Gold and Ogle Method)
Mean Melt Pt :  225.05 deg C (Joback; Gold,Ogle Methods)
  Selected MP:  183.35 deg C (Weighted Value)
-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   -5.10  |   -5.10
 Group | 18  |  -CH2-             |   11.27  |  202.86
 Group |  2  |  =CH-              |    8.73  |   17.46
 Group |  1  |  -C(=O)NH2         |  230.00  |  230.00
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  567.72
             |  MELTING POINT in deg C       |  294.56
-----------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: June 25, 2004
Order Number for Sorting:
Remarks:

2.1 MELTING POINT

Test Substance

Identity:	Dodecanamide, N-(2-hydroxyethyl)- (CAS RN 142-78-9)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Program (v 1.41) – The weighted mean was calculated using the values derived from the Joback Group Contribution Method and Gold and Ogle Method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Melting Point:	154 °C (weighted mean)
Decomposition:	Not applicable
Sublimation:	Not applicable
Remarks:	Following are the results from the model output (melting point only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(NCCO)CCCCCCCCCCC
CHEM   : Dodecanamide, N-(2-hydroxyethyl)-
MOL FOR: C14 H29 N1 O2
MOL WT : 243.39
---------------------- SUMMARY MPBPWIN v1.41 ------------------
Melting Point:  248.93 deg C (Adapted Joback Method)
Melting Point:  122.52 deg C (Gold and Ogle Method)
Mean Melt Pt :  185.72 deg C (Joback; Gold,Ogle Methods)
  Selected MP:  154.12 deg C (Weighted Value)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   -5.10  |   -5.10
 Group | 12  |  -CH2-             |   11.27  |  135.24
 Group |  1  |  -OH (primary)     |   44.45  |   44.45
 Group |  1  |  -C(=O)NH-         |  225.00  |  225.00
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  522.09
             |  MELTING POINT in deg C       |  248.93
-----------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: June 25, 2004
Order Number for Sorting:
Remarks:

2.1 MELTING POINT

Test Substance

Identity:	Dodecanamide, N,N-bis(2-hydroxyethyl)- (CAS RN 120-40-1)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	Standard reference book information; no experimental details provided.

Results

Melting point:	38.7 °C
Decomposition:	Not determined
Sublimation:	Not determined
Remarks:	

Conclusions

Remarks:	The melting point was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; secondary literature source.

References

Kirk-Othmer. Encyclopedia of Chemical Technology. (4)2. John Wiley & Sons, New York, NY, U. S.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	40
Remarks:	

2.1 MELTING POINT

Test Substance

Identity:	9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)- (CAS RN 93-83-4; Oleamide, N,N-bis(2-hydroxyethyl)-)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Program (v 1.41) – The weighted mean was calculated using the values derived from the Joback Group Contribution Method and Gold and Ogle Method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Melting Point:	204 °C (weighted mean)
Decomposition:	Not applicable
Sublimation:	Not applicable
Remarks:	Following are the results from the model output (melting point only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(N(CCO)CCO)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)-
MOL FOR: C22 H43 N1 O3
MOL WT : 369.59
--------------------- SUMMARY MPBPWIN v1.41 --------------------
Melting Point:  295.46 deg C (Adapted Joback Method)
Melting Point:  180.53 deg C (Gold and Ogle Method)
Mean Melt Pt :  237.99 deg C (Joback; Gold,Ogle Methods)
  Selected MP:  203.51 deg C (Weighted Value)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   -5.10  |   -5.10
 Group | 18  |  -CH2-             |   11.27  |  202.86
 Group |  2  |  =CH-              |    8.73  |   17.46
 Group |  2  |  -OH (primary)     |   44.45  |   88.90
 Group |  1  |  -C(=O)N<          |  142.00  |  142.00
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  568.62
             |  MELTING POINT in deg C       |  295.46
-----------------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.1 MELTING POINT

Test Substance

Identity:	Amides, C12-18, N,N-bis(hydroxyethyl) (CAS RN 68155-06-6)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Program (v 1.41) – The weighted mean was calculated using the values derived from the Joback Group Contribution Method and Gold and Ogle Method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Melting Point:	154 °C (weighted mean)
Decomposition:	Not applicable
Sublimation:	Not applicable
Remarks:	Following are the results from the model output (melting point only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(N(CCO)CCO)CCCCCCCCCC
CHEM   : Amides, C12-18, N,N-bis(hydroxyethyl)
MOL FOR: C15 H31 N1 O3
MOL WT : 273.42
---------------------- SUMMARY MPBPWIN v1.41 -------------------

Melting Point:  221.65 deg C (Adapted Joback Method)
Melting Point:  131.01 deg C (Gold and Ogle Method)
Mean Melt Pt :  176.33 deg C (Joback; Gold,Ogle Methods)
  Selected MP:  153.67 deg C (Weighted Value)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   -5.10  |   -5.10
 Group | 13  |  -CH2-             |   11.27  |  146.51
 Group |  2  |  -OH (primary)     |   44.45  |   88.90
 Group |  1  |  -C(=O)N<          |  142.00  |  142.00
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  494.81
             |  MELTING POINT in deg C       |  221.65
-----------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.1 MELTING POINT

Test Substance

Identity:	Octadecanamide, N,N'-1,2-ethanediylbis- (CAS RN 110-30-5; Octadecanamide, N,N'-ethylenebis)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Program (v 1.41) – The weighted mean was calculated using the values derived from the Joback Group Contribution Method and Gold and Ogle Method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Melting Point:	323 °C (weighted mean)
Decomposition:	Not applicable
Sublimation:	Not applicable
Remarks:	Following are the results from the model output (melting point only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(NCCNC(=O)CCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCC
CHEM   : Octadecanamide, N,N'-1,2-ethanediylbis-
MOL FOR: C38 H76 N2 O2
MOL WT : 593.04
--------------------- SUMMARY MPBPWIN v1.41 -------------------

Melting Point:  349.84 deg C (Adapted Joback Method)
Melting Point:  315.95 deg C (Gold and Ogle Method)
Mean Melt Pt :  332.89 deg C (Joback; Gold,Ogle Methods)
  Selected MP:  322.73 deg C (Weighted Value)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  2  |  -CH3              |   -5.10  |  -10.20
 Group | 34  |  -CH2-             |   11.27  |  383.18
 Group |  2  |  -C(=O)NH-         |  225.00  |  450.00
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  945.48
 RESULT-limit|  MELTING POINT in deg Kelvin  |  623.00
             |  MELTING POINT in deg C       |  349.84
-----------------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.2 BOILING POINT

Test Substance

Identity:	Stearamide (CAS RN 124-26-5)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	Standard reference book information; no experimental details provided.

Results

Boiling point:	250 – 251 °C at 12 mmHg
Decomposition:	Not determined
Sublimation:	Not determined
Remarks:	

Conclusions

Remarks:	The boiling point was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; secondary literature source.

References

Weast, R. C., (ed). 1979. CRC Handbook of Chemistry and Physics, 60th Edition. CRC Press, Boca Raton, FL, U. S.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	51
Remarks:	

2.2 BOILING POINT

Test Substance

Identity:	9-Octadecenamide, (Z)- (CAS RN 301-02-0; Oleamide)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the adapted Stein and Brown method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 76 °C.

Results

Boiling Point:	415 °C
Pressure:	760 mm Hg
Decomposition:	Not applicable
Remarks:	Following are the results from the model (boiling point only):

```
      MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(N)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenamide, (Z)-
MOL FOR: C18 H35 N1 O1
MOL WT : 281.49
---------------------- SUMMARY MPBPWIN v1.41 ------------------
Boiling Point:  414.63 deg C (Adapted Stein and Brown Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group | 14  |  -CH2-             |   24.22  |  339.08
 Group |  2  |  =CH-              |   27.95  |   55.90
 Group |  1  |  -C(=O)NH2         |  230.39  |  230.39
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  845.53
RESULT- corr |  BOILING POINT in deg Kelvin  |  687.79
             |  BOILING POINT in deg C       |  414.63
-----------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: June 25, 2004
Order Number for Sorting:
Remarks:

2.2 BOILING POINT

Test Substance

Identity:	13-Docosenamide, (Z)- (CAS RN 112-84-5; Erucamide)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the adapted Stein and Brown method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Boiling Point:	461 °C
Pressure:	760 mm Hg
Decomposition:	Not applicable
Remarks:	Following are the results from the model (boiling point only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match: no data

SMILES : O=C(N)CCCCCCCCCCCC=CCCCCCCCC
CHEM   : 13-Docosenamide, (Z)-
MOL FOR: C22 H43 N1 O1
MOL WT : 337.59

---------------------- SUMMARY MPBPWIN v1.41 -------------------
Boiling Point:  461.05 deg C (Adapted Stein and Brown Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group | 18  |  -CH2-             |   24.22  |  435.96
 Group |  2  |  =CH-              |   27.95  |   55.90
 Group |  1  |  -C(=O)NH2         |  230.39  |  230.39
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  942.41
RESULT- corr |  BOILING POINT in deg Kelvin  |  734.21
             |  BOILING POINT in deg C       |  461.05
-----------------------------------------------------------
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: June 25, 2004
Order Number for Sorting:
Remarks:

2.2 BOILING POINT

Test Substance

Identity:	Dodecanamide, N-(2-hydroxyethyl)- (CAS RN 142-78-9)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the adapted Stein and Brown method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Boiling Point:	404 °C
Pressure:	760 mm Hg
Decomposition:	Not applicable
Remarks:	Following are the results from the model (boiling point only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(NCCO)CCCCCCCCCCC
CHEM   : Dodecanamide, N-(2-hydroxyethyl)-
MOL FOR: C14 H29 N1 O2
MOL WT : 243.39
---------------------- SUMMARY MPBPWIN v1.41 --------------------
Boiling Point:  404.49 deg C (Adapted Stein and Brown Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group | 12  |  -CH2-             |   24.22  |  290.64
 Group |  1  |  -OH (primary)     |   88.46  |   88.46
 Group |  1  |  -C(=O)NH-         |  225.09  |  225.09
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  824.35
RESULT- corr |  BOILING POINT in deg Kelvin  |  677.65
             |  BOILING POINT in deg C       |  404.49
-------------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.2 BOILING POINT

Test Substance

Identity:	Dodecanamide, N,N-bis(2-hydroxyethyl)- (CAS RN 120-40-1)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the adapted Stein and Brown method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 38.7 °C.

Results

Boiling Point:	431 °C
Pressure:	760 mm Hg
Decomposition:	Not applicable
Remarks:	Following are the results from the model (boiling point only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:
  Name     :  N,N-DI(2-HYDROXYETHYL)LAURAMIDE
  CAS Num  :  000120-40-1
  Exp BP (deg C):  ---

SMILES : O=C(N(CCO)CCO)CCCCCCCCCCC
CHEM   : Dodecanamide, N,N-bis(2-hydroxyethyl)-
MOL FOR: C16 H33 N1 O3
MOL WT : 287.45
---------------------- SUMMARY MPBPWIN v1.41 --------------------
Boiling Point:  430.64 deg C (Adapted Stein and Brown Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group | 14  |  -CH2-             |   24.22  |  339.08
 Group |  2  |  -OH (primary)     |   88.46  |  176.92
 Group |  1  |  -C(=O)N<          |  142.77  |  142.77
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  878.93
RESULT- corr |  BOILING POINT in deg Kelvin  |  703.80
             |  BOILING POINT in deg C       |  430.64
-----------------------------------------------------
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.2 BOILING POINT

Test Substance

Identity:	9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)- (CAS RN 93-83-4; Oleamide, N,N-bis(2-hydroxyethyl)-)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the adapted Stein and Brown method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Boiling Point:	504 °C
Pressure:	760 mm Hg
Decomposition:	Not applicable
Remarks:	Following are the results from the model (boiling point only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(N(CCO)CCO)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)-
MOL FOR: C22 H43 N1 O3
MOL WT : 369.59
-------------------- SUMMARY MPBPWIN v1.41 ------------------
Boiling Point:  503.83 deg C (Adapted Stein and Brown Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group | 18  |  -CH2-             |   24.22  |  435.96
 Group |  2  |  =CH-              |   27.95  |   55.90
 Group |  2  |  -OH (primary)     |   88.46  |  176.92
 Group |  1  |  -C(=O)N<          |  142.77  |  142.77
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  | 1031.71
RESULT- corr |  BOILING POINT in deg Kelvin  |  776.99
             |  BOILING POINT in deg C       |  503.83
-----------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.2 BOILING POINT

Test Substance

Identity:	Amides, C12-18, N,N-bis(hydroxyethyl) (CAS RN 68155-06-6)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the adapted Stein and Brown method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Boiling Point:	419 °C
Pressure:	760 mm Hg
Decomposition:	Not applicable
Remarks:	Following are the results from the model (boiling point only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(N(CCO)CCO)CCCCCCCCCC
CHEM   : Amides, C12-18, N,N-bis(hydroxyethyl)
MOL FOR: C15 H31 N1 O3
MOL WT : 273.42
---------------------- SUMMARY MPBPWIN v1.41 --------------------

Boiling Point:  419.03 deg C (Adapted Stein and Brown Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group | 13  |  -CH2-             |   24.22  |  314.86
 Group |  2  |  -OH (primary)     |   88.46  |  176.92
 Group |  1  |  -C(=O)N<          |  142.77  |  142.77
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  854.71
RESULT- corr |  BOILING POINT in deg Kelvin  |  692.19
             |  BOILING POINT in deg C       |  419.03
-----------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.2 BOILING POINT

Test Substance

Identity:	Octadecanamide, N,N'-1,2-ethanediylbis- (CAS RN 110-30-5; Octadecanamide, N,N'-ethylenebis)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the adapted Stein and Brown method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Boiling Point:	736 °C
Pressure:	760 mm Hg
Decomposition:	Not applicable
Remarks:	Following are the results from the model (boiling point only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(NCCNC(=O)CCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCC
CHEM   : Octadecanamide, N,N'-1,2-ethanediylbis-
MOL FOR: C38 H76 N2 O2
MOL WT : 593.04
---------------------- SUMMARY MPBPWIN v1.41 --------------------

Boiling Point:  735.76 deg C (Adapted Stein and Brown Method)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  2  |  -CH3              |   21.98  |   43.96
 Group | 34  |  -CH2-             |   24.22  |  823.48
 Group |  2  |  -C(=O)NH-         |  225.09  |  450.18
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  | 1515.80
RESULT- corr |  BOILING POINT in deg Kelvin  | 1008.92
             |  BOILING POINT in deg C       |  735.76
-----------------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.4 VAPOR PRESSURE

Test Substance

Identity:	Octadecanamide (CAS RN 124-26-5; Stearamide)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the Modified Grain method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 109 °C and boiling point of 250 °C.

Results

Vapor Pressure:	0.004 mmHg
Temperature:	25°C
Decomposition:	Not applicable
Remarks:	Following are the results from the model (vapor pressure only):

```
     MPBPWIN (v1.41) Program Results:
==============================
Experimental Database Structure Match: No Data

SMILES : O=C(N)CCCCCCCCCCCCCCCC
CHEM   : Octadecanamide
MOL FOR: C18 H37 N1 O1
MOL WT : 283.50
---------------------- SUMMARY MPBPWIN v1.41 ------------------
Vapor Pressure Estimations (25 deg C):
  (Using BP: 250.00 deg C (user entered))
  (Using MP: 109.00 deg C (user entered))
    VP:  0.00417 mm Hg (Antoine Method)
    VP:  0.00398 mm Hg (Modified Grain Method)
    VP:  0.00692 mm Hg (Mackay Method)
  Selected VP:  0.00398 mm Hg (Modified Grain Method)
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: June 25, 2004
Order Number for Sorting:
Remarks:

2.4 VAPOR PRESSURE

Test Substance

Identity:	9-Octadecenamide, (Z)- (CAS RN 301-02-0; Oleamide)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the Modified Grain method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 76 °C.

Results

Vapor Pressure:	1.2 E-6 mmHg
Temperature:	25°C
Decomposition:	Not applicable
Remarks:	Following are the results from the model (vapor pressure only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(N)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenamide, (Z)-
MOL FOR: C18 H35 N1 O1
MOL WT : 281.49
---------------------- SUMMARY MPBPWIN v1.41 ------------------
Vapor Pressure Estimations (25 deg C):
  (Using BP: 414.63 deg C (estimated))
  (Using MP: 76.00 deg C (user entered))
    VP:  1.9E-007 mm Hg (Antoine Method)
    VP:  1.2E-006 mm Hg (Modified Grain Method)
    VP:  2.37E-006 mm Hg (Mackay Method)
  Selected VP:  1.2E-006 mm Hg (Modified Grain Method)
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: June 25, 2004
Order Number for Sorting:
Remarks:

2.4 VAPOR PRESSURE

Test Substance

Identity:	13-Docosenamide, (Z)- (CAS RN 112-84-5; Erucamide)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the Modified Grain method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Vapor Pressure:	8.3 E-8 mmHg
Temperature:	25°C
Decomposition:	Not applicable
Remarks:	Following are the results from the model (vapor pressure only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match: no data

SMILES : O=C(N)CCCCCCCCCCCC=CCCCCCCCC
CHEM   : 13-Docosenamide, (Z)-
MOL FOR: C22 H43 N1 O1
MOL WT : 337.59
---------------------- SUMMARY MPBPWIN v1.41 ------------------
Vapor Pressure Estimations (25 deg C):
  (Using BP: 461.05 deg C (estimated))
  (Using MP: 77.50 deg C (exp database))
    VP:  4.23E-009 mm Hg (Antoine Method)
    VP:  8.28E-008 mm Hg (Modified Grain Method)
    VP:  1.67E-007 mm Hg (Mackay Method)
  Selected VP:  8.28E-008 mm Hg (Modified Grain Method)
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: June 25, 2004
Order Number for Sorting:
Remarks:

2.4 VAPOR PRESSURE

Test Substance

Identity:	Dodecanamide, N-(2-hydroxyethyl)- (CAS RN 142-78-9)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the Modified Grain method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Vapor Pressure:	6.6 E-9 mmHg
Temperature:	25°C
Decomposition:	Not applicable
Remarks:	Following are the results from the model (vapor pressure only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(NCCO)CCCCCCCCCCC
CHEM   : Dodecanamide, N-(2-hydroxyethyl)-
MOL FOR: C14 H29 N1 O2
MOL WT : 243.39
---------------------- SUMMARY MPBPWIN v1.41 --------------------
Vapor Pressure Estimations (25 deg C):
  (Using BP: 404.49 deg C (estimated))
  (Using MP: 154.12 deg C (estimated))
    VP:  9.11E-010 mm Hg (Antoine Method)
    VP:  6.57E-009 mm Hg (Modified Grain Method)
    VP:  7.02E-007 mm Hg (Mackay Method)
  Selected VP:  6.57E-009 mm Hg (Modified Grain Method)
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.4 VAPOR PRESSURE

Test Substance

Identity:	Dodecanamide, N,N-bis(2-hydroxyethyl)- (CAS RN 120-40-1)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the Modified Grain method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 38.7 °C.

Results

Vapor Pressure:	6.7 E-9 mmHg
Temperature:	25°C
Decomposition:	Not applicable
Remarks:	Following are the results from the model (vapor pressure only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:
  Name     :  N,N-DI(2-HYDROXYETHYL)LAURAMIDE
  CAS Num  :  000120-40-1
  Exp VP (mm Hg):  ---

SMILES : O=C(N(CCO)CCO)CCCCCCCCCCC
CHEM   : Dodecanamide, N,N-bis(2-hydroxyethyl)-
MOL FOR: C16 H33 N1 O3
MOL WT : 287.45
---------------------- SUMMARY MPBPWIN v1.41 --------------------

Vapor Pressure Estimations (25 deg C):
  (Using BP: 430.64 deg C (estimated))
  (Using MP: 38.70 deg C (user entered))
    VP:  4.29E-010 mm Hg (Antoine Method)
    VP:  6.73E-009 mm Hg (Modified Grain Method)
    VP:  2.26E-006 mm Hg (Mackay Method)
  Selected VP:  6.73E-009 mm Hg (Modified Grain Method)
```

Conclusions	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed:	July 6, 2004
Order Number for Sorting:	
Remarks:	

2.4 VAPOR PRESSURE

Test Substance

Identity:	9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)- (CAS RN 93-83-4, Oleamide, N,N-bis(2-hydroxyethyl)-)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the Modified Grain method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Vapor Pressure:	5.9 E-13 mmHg
Temperature:	25°C
Decomposition:	Not applicable
Remarks:	Following are the results from the model (vapor pressure only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(N(CCO)CCO)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)-
MOL FOR: C22 H43 N1 O3
MOL WT : 369.59
---------------------- SUMMARY MPBPWIN v1.41 --------------------

Vapor Pressure Estimations (25 deg C):
  (Using BP: 503.83 deg C (estimated))
  (Using MP: 203.51 deg C (estimated))
    VP:  2.54E-015 mm Hg (Antoine Method)
    VP:  5.88E-013 mm Hg (Modified Grain Method)
    VP:  8E-010 mm Hg (Mackay Method)
Selected VP:  5.88E-013 mm Hg (Modified Grain Method)
```

Conclusions	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.4 VAPOR PRESSURE

Test Substance

Identity:	Amides, C12-18, N,N-bis(hydroxyethyl) (CAS RN 68155-06-6)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the Modified Grain method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Vapor Pressure:	1 E-09 mmHg
Temperature:	25°C
Decomposition:	Not applicable
Remarks:	Following are the results from the model (vapor pressure only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(N(CCO)CCO)CCCCCCCCCC
CHEM   : Amides, C12-18, N,N-bis(hydroxyethyl)
MOL FOR: C15 H31 N1 O3
MOL WT : 273.42
---------------------- SUMMARY MPBPWIN v1.41 --------------------

Vapor Pressure Estimations (25 deg C):
  (Using BP: 419.03 deg C (estimated))
  (Using MP: 153.67 deg C (estimated))
    VP:  8.75E-011 mm Hg (Antoine Method)
    VP:  9.91E-010 mm Hg (Modified Grain Method)
    VP:  3.15E-007 mm Hg (Mackay Method)
  Selected VP:  9.91E-010 mm Hg (Modified Grain Method)
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.4 VAPOR PRESSURE

Test Substance

Identity:	Octadecanamide, N,N'-1,2-ethanediylbis- (CAS RN 110-30-5; Octadecanamide, N,N'-ethylenebis)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the Modified Grain method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Vapor Pressure:	8 E-18 mmHg
Temperature:	25°C
Decomposition:	Not applicable
Remarks:	Following are the results from the model (vapor pressure only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(NCCNC(=O)CCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCC
CHEM   : Octadecanamide, N,N'-1,2-ethanediylbis-
MOL FOR: C38 H76 N2 O2
MOL WT : 593.04
---------------------- SUMMARY MPBPWIN v1.41 ------------------

Vapor Pressure Estimations (25 deg C):
  (Using BP: 735.76 deg C (estimated))
  (Using MP: 322.73 deg C (estimated))
    VP:  1.33E-026 mm Hg (Antoine Method)
    VP:  7.97E-018 mm Hg (Modified Grain Method)
    VP:  4.16E-017 mm Hg (Mackay Method)
  Selected VP:  7.97E-018 mm Hg (Modified Grain Method)
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	Octadecanamide (CAS RN 124-26-5; Stearamide)
Purity:	Not applicable

Method

Method:	EPIWIN (v 3.11), KOWWIN Program (v 1.67)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 109 °C and boiling point of 250 °C.

Results

Log K_{ow}:	6.70
Temperature °C:	Not stated
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.67) Results:
===============================

                  Log Kow(version 1.67 estimate): 6.70

SMILES : O=C(N)CCCCCCCCCCCCCCCC
CHEM   : Octadecanamide
MOL FOR: C18 H37 N1 O1
MOL WT : 283.50
-------+-----+-------------------------------------+---------+--------
 TYPE  | NUM |        LOGKOW FRAGMENT DESCRIPTION  |  COEFF  |  VALUE
-------+-----+-------------------------------------+---------+--------
 Frag  |  1  |  -CH3    [aliphatic carbon]         | 0.5473  |  0.5473
 Frag  | 16  |  -CH2-   [aliphatic carbon]         | 0.4911  |  7.8576
 Frag  |  1  |  -NH2    [aliphatic attach]         |-1.4148  | -1.4148
 Frag  |  1  |  -C(=O)N  [aliphatic attach]        |-0.5236  | -0.5236
 Const |     |  Equation Constant                  |         |  0.2290
-------+-----+-------------------------------------+---------+--------
                                                  Log Kow   =   6.6955
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; KOWWIN Program, Version 1.67; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: June 25, 2004
Order Number for Sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	9-Octadecenamide, (Z)- (CAS RN 301-02-0; Oleamide)
Purity:	Not applicable

Method

Method:	EPIWIN (v 3.11), KOWWIN Program (v 1.67)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 76 °C.

Results

Log K_{ow}:	6.48
Temperature °C:	Not stated
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.67) Results:
===============================

                  Log Kow(version 1.67 estimate): 6.48

SMILES : O=C(N)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenamide, (Z)-
MOL FOR: C18 H35 N1 O1
MOL WT : 281.49
-------+-----+---------------------------------------+---------+--------
 TYPE  | NUM |     LOGKOW FRAGMENT DESCRIPTION       |  COEFF  |  VALUE
-------+-----+---------------------------------------+---------+--------
 Frag  |  1  |  -CH3    [aliphatic carbon]           | 0.5473  |  0.5473
 Frag  | 14  |  -CH2-   [aliphatic carbon]           | 0.4911  |  6.8754
 Frag  |  2  |  =CH- or =C<  [olefinc carbon]        | 0.3836  |  0.7672
 Frag  |  1  |  -NH2    [aliphatic attach]           |-1.4148  | -1.4148
 Frag  |  1  |  -C(=O)N  [aliphatic attach]          |-0.5236  | -0.5236
 Const |     |  Equation Constant                    |         |  0.2290
-------+-----+---------------------------------------+---------+--------
                                                  Log Kow   =   6.4805
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; KOWWIN Program, Version

1.67; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: June 25, 2004
Order Number for Sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	13-Docosenamide, (Z)- (CAS RN 112-84-5; Erucamide)
Purity:	Not applicable

Method

Method:	EPIWIN (v 3.11), KOWWIN Program (v 1.67)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Log K_{ow}:	8.44
Temperature °C:	Not stated
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.67) Results:
==============================

                  Log Kow(version 1.67 estimate): 8.44

SMILES : O=C(N)CCCCCCCCCCCC=CCCCCCCCC
CHEM   : 13-Docosenamide, (Z)-
MOL FOR: C22 H43 N1 O1
MOL WT : 337.59
-------+-----+---------------------------------------+---------+--------
 TYPE  | NUM |       LOGKOW FRAGMENT DESCRIPTION     |  COEFF  |  VALUE
-------+-----+---------------------------------------+---------+--------
 Frag  |  1  |  -CH3    [aliphatic carbon]           | 0.5473  |  0.5473
 Frag  | 18  |  -CH2-   [aliphatic carbon]           | 0.4911  |  8.8398
 Frag  |  2  |  =CH- or =C<  [olefinc carbon]        | 0.3836  |  0.7672
 Frag  |  1  |  -NH2    [aliphatic attach]           |-1.4148  | -1.4148
 Frag  |  1  |  -C(=O)N  [aliphatic attach]          |-0.5236  | -0.5236
 Const |     |  Equation Constant                    |         |  0.2290
-------+-----+---------------------------------------+---------+--------
                                                  Log Kow   =   8.4449
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; KOWWIN Program, Version 1.67; PC-Computer software developed by EPA's Office of

Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: June 25, 2004
Order Number for Sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	Dodecanamide, N-(2-hydroxyethyl)- (CAS RN 142-78-9)
Purity:	Not applicable

Method

Method:	EPIWIN (v 3.11), KOWWIN Program (v 1.67)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Log K_{ow}:	3.24
Temperature °C:	Not stated
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.67) Results:
===============================

                  Log Kow(version 1.67 estimate): 3.24

SMILES : O=C(NCCO)CCCCCCCCCCC
CHEM   : Dodecanamide, N-(2-hydroxyethyl)-
MOL FOR: C14 H29 N1 O2
MOL WT : 243.39
-------+-----+---------------------------------------+---------+--------
 TYPE  | NUM |       LOGKOW FRAGMENT DESCRIPTION     |  COEFF  |  VALUE
-------+-----+---------------------------------------+---------+--------
 Frag  |  1  |  -CH3    [aliphatic carbon]           | 0.5473  |  0.5473
 Frag  | 12  |  -CH2-   [aliphatic carbon]           | 0.4911  |  5.8932
 Frag  |  1  |  -OH     [hydroxy, aliphatic attach]  |-1.4086  | -1.4086
 Frag  |  1  |  -NH-    [aliphatic attach]           |-1.4962  | -1.4962
 Frag  |  1  |  -C(=O)N  [aliphatic attach]          |-0.5236  | -0.5236
 Const |     |  Equation Constant                    |         |  0.2290
-------+-----+---------------------------------------+---------+--------
                                                   Log Kow   =   3.2411
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; KOWWIN Program, Version 1.67; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	Dodecanamide, N,N-bis(2-hydroxyethyl)- (CAS RN 120-40-1)
Purity:	Not applicable

Method

Method:	EPIWIN (v 3.11), KOWWIN Program (v 1.67)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 38.7 °C.

Results

Log K_{ow}:	2.89
Temperature °C:	Not stated
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.67) Results:
===============================

                  Log Kow(version 1.67 estimate): 2.89

SMILES : O=C(N(CCO)CCO)CCCCCCCCCCC
CHEM   : Dodecanamide, N,N-bis(2-hydroxyethyl)-
MOL FOR: C16 H33 N1 O3
MOL WT : 287.45
-------+-----+--------------------------------------+---------+--------
 TYPE  | NUM |      LOGKOW FRAGMENT DESCRIPTION     | COEFF   | VALUE
-------+-----+--------------------------------------+---------+--------
 Frag  |  1  |  -CH3    [aliphatic carbon]          | 0.5473  |  0.5473
 Frag  | 14  |  -CH2-   [aliphatic carbon]          | 0.4911  |  6.8754
 Frag  |  2  |  -OH     [hydroxy, aliphatic attach] |-1.4086  | -2.8172
 Frag  |  1  |  -N<     [aliphatic attach]          |-1.8323  | -1.8323
 Frag  |  1  |  -C(=O)N  [aliphatic attach]         |-0.5236  | -0.5236
 Factor|  1  |  Multi-alcohol correction            | 0.4064  |  0.4064
 Const |     |  Equation Constant                   |         |  0.2290
-------+-----+--------------------------------------+---------+--------
                                                  Log Kow   =   2.8850
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; KOWWIN Program, Version 1.67; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)- (CAS RN 93-83-4, Oleamide, N,N-bis(2-hydroxyethyl)-)
Purity:	Not applicable

Method

Method:	EPIWIN (v 3.11), KOWWIN Program (v 1.67)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Log K_{ow}:	5.62
Temperature °C:	Not stated
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.67) Results:
===============================

                  Log Kow(version 1.67 estimate): 5.62

SMILES : O=C(N(CCO)CCO)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)-
MOL FOR: C22 H43 N1 O3
MOL WT : 369.59
-------+-----+---------------------------------------+---------+--------
 TYPE  | NUM |      LOGKOW FRAGMENT DESCRIPTION      | COEFF   |  VALUE
-------+-----+---------------------------------------+---------+--------
 Frag  |  1  |  -CH3    [aliphatic carbon]           | 0.5473  |  0.5473
 Frag  | 18  |  -CH2-   [aliphatic carbon]           | 0.4911  |  8.8398
 Frag  |  2  |  =CH- or =C<  [olefinc carbon]        | 0.3836  |  0.7672
 Frag  |  2  |  -OH     [hydroxy, aliphatic attach]  |-1.4086  | -2.8172
 Frag  |  1  |  -N<     [aliphatic attach]           |-1.8323  | -1.8323
 Frag  |  1  |  -C(=O)N  [aliphatic attach]          |-0.5236  | -0.5236
 Factor|  1  |  Multi-alcohol correction             | 0.4064  |  0.4064
 Const |     |  Equation Constant                    |         |  0.2290
-------+-----+---------------------------------------+---------+--------
                                                 Log Kow   =   5.6166
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; KOWWIN Program, Version 1.67; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	Amides, C12-18, N,N-bis(hydroxyethyl) (CAS RN 68155-06-6)
Purity:	Not applicable

Method

Method:	EPIWIN (v 3.11), KOWWIN Program (v 1.67)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Log K_{ow}:	2.39
Temperature °C:	Not stated
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.67) Results:
===============================

                  Log Kow(version 1.67 estimate): 2.39

SMILES : O=C(N(CCO)CCO)CCCCCCCCCC
CHEM   : Amides, C12-18, N,N-bis(hydroxyethyl)
MOL FOR: C15 H31 N1 O3
MOL WT : 273.42
-------+-----+--------------------------------------+---------+--------
 TYPE  | NUM |     LOGKOW FRAGMENT DESCRIPTION      | COEFF   |  VALUE
-------+-----+--------------------------------------+---------+--------
 Frag  |  1  |  -CH3    [aliphatic carbon]          | 0.5473  |  0.5473
 Frag  | 13  |  -CH2-   [aliphatic carbon]          | 0.4911  |  6.3843
 Frag  |  2  |  -OH     [hydroxy, aliphatic attach] |-1.4086  | -2.8172
 Frag  |  1  |  -N<     [aliphatic attach]          |-1.8323  | -1.8323
 Frag  |  1  |  -C(=O)N  [aliphatic attach]         |-0.5236  | -0.5236
 Factor|  1  |  Multi-alcohol correction            | 0.4064  |  0.4064
 Const |     |  Equation Constant                   |         |  0.2290
-------+-----+--------------------------------------+---------+--------
                                                  Log Kow   =   2.3939
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; KOWWIN Program, Version 1.67; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	Octadecanamide, N,N'-1,2-ethanediylbis- (CAS RN 110-30-5; Octadecanamide, N,N'-ethylenebis)
Purity:	Not applicable

Method

Method:	EPIWIN (v 3.11), KOWWIN Program (v 1.67)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Log K_{ow}:	13.98
Temperature °C:	Not stated
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.67) Results:
===============================

                  Log Kow(version 1.67 estimate): 13.98

SMILES : O=C(NCCNC(=O)CCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCC
CHEM   : Octadecanamide, N,N'-1,2-ethanediylbis-
MOL FOR: C38 H76 N2 O2
MOL WT : 593.04
-------+-----+---------------------------------------+---------+--------
 TYPE  | NUM |        LOGKOW FRAGMENT DESCRIPTION    | COEFF   |  VALUE
-------+-----+---------------------------------------+---------+--------
 Frag  |  2  |  -CH3    [aliphatic carbon]           | 0.5473  |  1.0946
 Frag  | 34  |  -CH2-   [aliphatic carbon]           | 0.4911  | 16.6974
 Frag  |  2  |  -NH-    [aliphatic attach]           |-1.4962  | -2.9924
 Frag  |  2  |  -C(=O)N  [aliphatic attach]          |-0.5236  | -1.0472
 Const |     |  Equation Constant                    |         |  0.2290
-------+-----+---------------------------------------+---------+--------
                                                    Log Kow   =  13.9814
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; KOWWIN Program, Version

1.67; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.6 WATER SOLUBILITY

Test Substance

Identity:	Stearamide (CAS RN 124-26-5)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	Standard reference book information; no experimental details provided.

Results

Water Solubility:	Insoluble in water
Decomposition:	Not determined
Sublimation:	Not determined
Remarks:	

Conclusions

Remarks:	Water solubility was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; secondary literature source.

References

Weast, R. C., (ed). 1979. CRC Handbook of Chemistry and Physics, 60th Edition. CRC Press, Boca Raton, FL, U. S.

Other Available Reports

Other

Last changed:	August 1, 2000
Order number for sorting:	51
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	Oleamide (CAS RN 301-02-0)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	Standard reference book information; no experimental details provided.

Results

Water Solubility:	Insoluble in water
Decomposition:	Not determined
Sublimation:	Not determined
Remarks:	

Conclusions

Remarks:	Water solubility was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; secondary literature source.

References

Weast, R. C. and M. J. Astle, (eds). 1980. CRC Handbook of Chemistry and Physics, 60th Edition. CRC Press, Boca Raton, FL, U. S.

Other Available Reports

Other

Last changed:	August 1, 2000
Order number for sorting:	74
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	13-Docosenamide, (Z)- (CAS RN 112-84-5; Erucamide)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11), WSKOWWIN Program (v 1.41)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Solubility:	0.0005 mg/L
Temperature:	25°C
pH value and concentration:	Not stated
pKa value at 25°C:	Not stated
Remarks:	Following are the results from the model:

```
Water Sol from Kow (WSKOW v1.41) Results:
=========================================

          Water Sol: 0.0004516 mg/L

SMILES : O=C(N)CCCCCCCCCCCC=CCCCCCCCC
CHEM   : 13-Docosenamide, (Z)-
MOL FOR: C22 H43 N1 O1
MOL WT : 337.59
---------------------- WSKOW v1.41 Results ------------------
Log Kow  (estimated)  :  8.44
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  8.44

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      --------------------   -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -8.874
   Water Solubility at 25 deg C (mg/L):  0.0004516
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; WSKOWWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed:	June 25, 2004
Order Number for Sorting:	
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	Dodecanamide, N-(2-hydroxyethyl)- (CAS RN 142-78-9)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11), WSKOWWIN Program (v 1.41)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Solubility:	43.9 mg/L
Temperature:	25°C
pH value and concentration:	Not stated
pKa value at 25°C:	Not stated
Remarks:	Following are the results from the model:

```
Water Sol from Kow (WSKOW v1.41) Results:
=========================================

          Water Sol: 43.9 mg/L

SMILES : O=C(NCCO)CCCCCCCCCCC
CHEM   : Dodecanamide, N-(2-hydroxyethyl)-
MOL FOR: C14 H29 N1 O2
MOL WT : 243.39
--------------- WSKOW v1.41 Results -------------
Log Kow  (estimated)  :  3.24
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  3.24

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      -------------------    -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -3.744
   Water Solubility at 25 deg C (mg/L):  43.9
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; WSKOWWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 6, 2004
Order Number for Sorting:
Remarks:

2.6 WATER SOLUBILITY

Test Substance

Identity:	Standamid LDO (CAS RN 120-40-1; Dodecanamide, N,N-bis(2-hydroxyethyl)-)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
GLP:	Not stated
Year:	Not stated
Remarks:	Standard reference book information; no experimental details provided.

Results

Water Solubility:	Insoluble in water.
Decomposition:	Not determined
Sublimation:	Not determined
Remarks:	

Conclusions

Remarks:	Water solubility was provided in a reliable resource book. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; secondary literature source.

References

Ash, M. and I. Ash. Encyclopedia of Surfactants. Volume IV. p. 397. Chemical Publishing Co., New York, NY.

Other Available Reports

Other

Last changed:	July 2, 2001
Order number for sorting:	41
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)- (CAS RN 93-83-4, Oleamide, N,N-bis(2-hydroxyethyl)-)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11), WSKOWWIN Program (v 1.41)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Solubility:	0.08 mg/L
Temperature:	25°C
pH value and concentration:	Not stated
pKa value at 25°C:	Not stated
Remarks:	Following are the results from the model:

```
Water Sol from Kow (WSKOW v1.41) Results:
=========================================

          Water Sol: 0.07525 mg/L

SMILES : O=C(N(CCO)CCO)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)-
MOL FOR: C22 H43 N1 O3
MOL WT : 369.59
------------------------- WSKOW v1.41 Results -----------------------
Log Kow  (estimated)  :  5.62
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  5.62

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      -------------------    -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -6.691
      Water Solubility at 25 deg C (mg/L):  0.07525
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; WSKOWWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed:	July 6, 2004
Order Number for Sorting:	
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	Amides, C12-18, N,N-bis(hydroxyethyl) (CAS RN 68155-06-6)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11), WSKOWWIN Program (v 1.41)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Solubility:	158 mg/L
Temperature:	25°C
pH value and concentration:	Not stated
pKa value at 25°C:	Not stated
Remarks:	Following are the results from the model:

```
Water Sol from Kow (WSKOW v1.41) Results:
=========================================

          Water Sol: 157.7 mg/L

SMILES : O=C(N(CCO)CCO)CCCCCCCCC
CHEM   : Amides, C12-18, N,N-bis(hydroxyethyl)
MOL FOR: C15 H31 N1 O3
MOL WT : 273.42
---------------------- WSKOW v1.41 Results ----------------------
Log Kow  (estimated)  :  2.39
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  2.39

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      -------------------    -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -3.239
   Water Solubility at 25 deg C (mg/L):  157.7
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; WSKOWWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed:	July 6, 2004
Order Number for Sorting:	
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	Octadecanamide, N,N'-1,2-ethanediylbis- (CAS RN 110-30-5; Octadecanamide, N,N'-ethylenebis)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11), WSKOWWIN Program (v 1.41)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Solubility:	2.0 E-10 mg/L
Temperature:	25°C
pH value and concentration:	Not stated
pKa value at 25°C:	Not stated
Remarks:	Following are the results from the model:

```
Water Sol from Kow (WSKOW v1.41) Results:
=========================================

          Water Sol: 2.049e-010 mg/L

SMILES : O=C(NCCNC(=O)CCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCC
CHEM   : Octadecanamide, N,N'-1,2-ethanediylbis-
MOL FOR: C38 H76 N2 O2
MOL WT : 593.04
---------------------- WSKOW v1.41 Results ----------------------
Log Kow  (estimated)  :  13.98
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  13.98

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      -------------------    -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -15.461
   Water Solubility at 25 deg C (mg/L):  2.049e-010
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; WSKOWWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed:	July 6, 2004
Order Number for Sorting:	
Remarks:	

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	Octadecanamide (CAS RN 124-26-5; Stearamide)
Purity:	Not applicable

Method

Method/guideline followed:	EPIWIN (v 3.11), AOPWIN Program (v 1.91)
Type:	Not applicable
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 109 °C and boiling point of 250 °C.

Results

Concentration of substance:	Not applicable
Temperature (°C):	Not stated
Direct photolysis:	Not stated
Indirect photolysis:	Not stated
Breakdown products:	Not applicable
Remarks:	Overall OH Rate Constant: (k_{phot}) = 27 E-12 cm^3/molecule-sec; Half life: $t_{1/2}$ = 4.7 hrs

Following are the results from the model:

```
AOP Program (v1.91) Results:
============================
SMILES : O=C(N)CCCCCCCCCCCCCCCCC
CHEM   : Octadecanamide
MOL FOR: C18 H37 N1 O1
MOL WT : 283.50
------------ SUMMARY (AOP v1.91): HYDROXYL RADICALS ------------
Hydrogen Abstraction       =  25.0277 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   2.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  27.0277 E-12 cm3/molecule-sec
   HALF-LIFE =     0.396 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =     4.749 Hrs
------------ SUMMARY (AOP v1.91): OZONE REACTION --------------

               ******  NO OZONE REACTION ESTIMATION ******
               (ONLY Olefins and Acetylenes are Estimated)
```

Experimental Database: NO Structure Matches

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; AOPWIN Program, Version 1.91; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: June 25, 2004
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	9-Octadecenamide, (Z)- (CAS RN 301-02-0; Oleamide)
Purity:	Not applicable

Method

Method/guideline followed:	EPIWIN (v 3.11), AOPWIN Program (v 1.91)
Type:	Not applicable
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 76 °C.

Results

Concentration of substance:	Not applicable
Temperature (°C):	Not stated
Direct photolysis:	Not stated
Indirect photolysis:	Not stated
Breakdown products:	Not applicable
Remarks:	Overall OH Rate Constant: (k_{phot}) = 80 E-12 cm^3/molecule-sec [Cis-isomer] (k_{phot}) = 88 E-12 cm^3/molecule-sec [Trans-isomer] Half-life: $t_{1/2}$ [Cis-isomer] = 1.6 hrs $t_{1/2}$ [Trans-isomer] = 1.5 hrs Following are the results from the model:

```
AOP Program (v1.91) Results:
============================
SMILES : O=C(N)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenamide, (Z)-
MOL FOR: C18 H35 N1 O1
MOL WT : 281.49
--------------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ---------------
Hydrogen Abstraction       =  21.6732 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   2.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =  56.4000 E-12 cm3/molecule-sec [Cis-isomer]
Addition to Olefinic Bonds =  64.0000 E-12 cm3/molecule-sec [Trans-isomer]
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

  OVERALL OH Rate Constant =  80.0732 E-12 cm3/molecule-sec [Cis-isomer]
  OVERALL OH Rate Constant =  87.6732 E-12 cm3/molecule-sec [Trans-isomer]
  HALF-LIFE =    1.603 Hrs (12-hr day; 1.5E6 OH/cm3) [Cis-isomer]
  HALF-LIFE =    1.464 Hrs (12-hr day; 1.5E6 OH/cm3) [Trans-isomer]
--------------- SUMMARY (AOP v1.91): OZONE REACTION -----------------
```

```
  OVERALL OZONE Rate Constant =  13.000000 E-17 cm3/molecule-sec [Cis-]
  OVERALL OZONE Rate Constant =  20.000000 E-17 cm3/molecule-sec [Trans-]
  HALF-LIFE =  2.116 Hrs (at 7E11 mol/cm3) [Cis-isomer]
  HALF-LIFE =  1.375 Hrs (at 7E11 mol/cm3) [Trans-isomer]

 NOTE: Reaction with Nitrate Radicals May Be Important!

  Experimental Database:  NO Structure Matches
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; AOPWIN Program, Version 1.91; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: June 25, 2004
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	13-Docosenamide, (Z)- (CAS RN 112-84-5; Erucamide)
Purity:	Not applicable

Method

Method/guideline followed:	EPIWIN (v 3.11), AOPWIN Program (v 1.91)
Type:	Not applicable
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Concentration of substance:	Not applicable
Temperature (°C):	Not stated
Direct photolysis:	Not stated
Indirect photolysis:	Not stated
Breakdown products:	Not applicable
Remarks:	Overall OH Rate Constant: (k_{phot}) = 86 E-12 cm^3/molecule-sec [Cis-isomer] (k_{phot}) = 93 E-12 cm^3/molecule-sec [Trans-isomer] Half-life: $t_{1/2}$ [Cis-isomer] = 1.5 hrs $t_{1/2}$ [Trans-isomer] = 1.4 hrs Following are the results from the model:

```
AOP Program (v1.91) Results:
============================
SMILES : O=C(N)CCCCCCCCCCCC=CCCCCCCCC
CHEM   : 13-Docosenamide, (Z)-
MOL FOR: C22 H43 N1 O1
MOL WT : 337.59
--------------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ----------------
Hydrogen Abstraction       =  27.3254 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   2.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =  56.4000 E-12 cm3/molecule-sec [Cis-isomer]
Addition to Olefinic Bonds =  64.0000 E-12 cm3/molecule-sec [Trans-isomer]
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

  OVERALL OH Rate Constant =  85.7254 E-12 cm3/molecule-sec [Cis-isomer]
  OVERALL OH Rate Constant =  93.3254 E-12 cm3/molecule-sec [Trans-isomer]
   HALF-LIFE =    1.497 Hrs (12-hr day; 1.5E6 OH/cm3) [Cis-isomer]
   HALF-LIFE =    1.375 Hrs (12-hr day; 1.5E6 OH/cm3) [Trans-isomer]
---------------- SUMMARY (AOP v1.91): OZONE REACTION ------------------
```

```
  OVERALL OZONE Rate Constant =  13.000000 E-17 cm3/molecule-sec [Cis-]
  OVERALL OZONE Rate Constant =  20.000000 E-17 cm3/molecule-sec [Trans-]
   HALF-LIFE =  2.116 Hrs (at 7E11 mol/cm3) [Cis-isomer]
   HALF-LIFE =  1.375 Hrs (at 7E11 mol/cm3) [Trans-isomer]

 NOTE: Reaction with Nitrate Radicals May Be Important!

    Experimental Database:  NO Structure Matches
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; AOPWIN Program, Version 1.91; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: June 25, 2004
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	Dodecanamide, N-(2-hydroxyethyl)- (CAS RN 142-78-9)
Purity:	Not applicable

Method

Method/guideline followed:	EPIWIN (v 3.11), AOPWIN Program (v 1.91)
Type:	Not applicable
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Concentration of substance:	Not applicable
Temperature (°C):	Not stated
Direct photolysis:	Not stated
Indirect photolysis:	Not stated
Breakdown products:	Not applicable
Remarks:	Overall OH Rate Constant: (k_{phot}) = 31 E-12 cm^3/molecule-sec; Half life: $t_{1/2}$ = 4.2 hrs

Following are the results from the model:

```
AOP Program (v1.91) Results:
============================
SMILES : O=C(NCCO)CCCCCCCCCCC
CHEM   : Dodecanamide, N-(2-hydroxyethyl)-
MOL FOR: C14 H29 N1 O2
MOL WT : 243.39
----------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ------------------
Hydrogen Abstraction       =  25.2805 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   5.6400 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  30.9205 E-12 cm3/molecule-sec
   HALF-LIFE =     0.346 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =     4.151 Hrs
-------------- SUMMARY (AOP v1.91): OZONE REACTION -----------------

                  ****** NO OZONE REACTION ESTIMATION ******
                 (ONLY Olefins and Acetylenes are Estimated)

Experimental Database:  NO Structure Matches
```

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; AOPWIN Program, Version 1.91; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: July 6, 2004
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	Dodecanamide, N,N-bis(2-hydroxyethyl)- (CAS RN 120-40-1)
Purity:	Not applicable

Method

Method/guideline followed:	EPIWIN (v 3.11), AOPWIN Program (v 1.91)
Type:	Not applicable
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 38.7 °C.

Results

Concentration of substance:	Not applicable
Temperature (°C):	Not stated
Direct photolysis:	Not stated
Indirect photolysis:	Not stated
Breakdown products:	Not applicable
Remarks:	Overall OH Rate Constant: (k_{phot}) = 49 E-12 cm^3/molecule-sec; Half-life: $t_{1/2}$ = 2.6 hrs

Following are the results from the model:

```
AOP Program (v1.91) Results:
============================
SMILES : O=C(N(CCO)CCO)CCCCCCCCCCC
CHEM   : Dodecanamide, N,N-bis(2-hydroxyethyl)-
MOL FOR: C16 H33 N1 O3
MOL WT : 287.45
------------- SUMMARY (AOP v1.91): HYDROXYL RADICALS -----------------
Hydrogen Abstraction       =  34.0115 E-12 cm3/molecule-sec
Reaction with N, S and -OH =  15.2800 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  49.2915 E-12 cm3/molecule-sec
   HALF-LIFE =     0.217 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =     2.604 Hrs
------------- SUMMARY (AOP v1.91): OZONE REACTION --------------------

                  ****** NO OZONE REACTION ESTIMATION ******
                 (ONLY Olefins and Acetylenes are Estimated)

Experimental Database:  NO Structure Matches
```

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; AOPWIN Program, Version 1.91; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: July 6, 2004
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)- (CAS RN 93-83-4, Oleamide, N,N-bis(2-hydroxyethyl)-)
Purity:	Not applicable

Method

Method/guideline followed:	EPIWIN (v 3.11), AOPWIN Program (v 1.91)
Type:	Not applicable
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Concentration of substance:	Not applicable
Temperature (°C):	Not stated
Direct photolysis:	Not stated
Indirect photolysis:	Not stated
Breakdown products:	Not applicable
Remarks:	Overall OH Rate Constant: (k_{phot}) = 111 E-12 cm^3/molecule-sec [Cis-isomer] (k_{phot}) = 118 E-12 cm^3/molecule-sec [Trans-isomer] Half-life: $t_{1/2}$ [Cis-isomer] = 1.2 hrs $t_{1/2}$ [Trans-isomer] = 1.1 hrs Following are the results from the model:

```
AOP Program (v1.91) Results:
============================
SMILES : O=C(N(CCO)CCO)CCCCCCCC=CCCCCCCCC
CHEM   : 9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)-
MOL FOR: C22 H43 N1 O3
MOL WT : 369.59
--------------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ---------------
Hydrogen Abstraction       =  39.1352 E-12 cm3/molecule-sec
Reaction with N, S and -OH =  15.2800 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =  56.4000 E-12 cm3/molecule-sec [Cis-isomer]
Addition to Olefinic Bonds =  64.0000 E-12 cm3/molecule-sec [Trans-isomer]
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 110.8152 E-12 cm3/molecule-sec [Cis-isomer]
OVERALL OH Rate Constant = 118.4152 E-12 cm3/molecule-sec [Trans-isomer]
   HALF-LIFE =    1.158 Hrs (12-hr day; 1.5E6 OH/cm3) [Cis-isomer]
```

```
   HALF-LIFE =    1.084 Hrs (12-hr day; 1.5E6 OH/cm3) [Trans-isomer]
--------------- SUMMARY (AOP v1.91): OZONE REACTION --------------------
   OVERALL OZONE Rate Constant =  13.000000 E-17 cm3/molecule-sec [Cis-]
   OVERALL OZONE Rate Constant =  20.000000 E-17 cm3/molecule-sec [Trans-]
   HALF-LIFE =  2.116 Hrs (at 7E11 mol/cm3) [Cis-isomer]
   HALF-LIFE =  1.375 Hrs (at 7E11 mol/cm3) [Trans-isomer]

 NOTE: Reaction with Nitrate Radicals May Be Important!

Experimental Database:  NO Structure Matches
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; AOPWIN Program, Version 1.91; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: July 6, 2004
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	Amides, C12-18, N,N-bis(hydroxyethyl) (CAS RN 68155-06-6)
Purity:	Not applicable

Method

Method/guideline followed:	EPIWIN (v 3.11), AOPWIN Program (v 1.91)
Type:	Not applicable
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Concentration of substance:	Not applicable
Temperature (°C):	Not stated
Direct photolysis:	Not stated
Indirect photolysis:	Not stated
Breakdown products:	Not applicable
Remarks:	Overall OH Rate Constant: (k_{phot}) = 48 E-12 cm^3/molecule-sec; Half-life: $t_{1/2}$ = 2.7 hrs

Following are the results from the model:

```
AOP Program (v1.91) Results:
============================
SMILES : O=C(N(CCO)CCO)CCCCCCCCC
CHEM   : Amides, C12-18, N,N-bis(hydroxyethyl)
MOL FOR: C15 H31 N1 O3
MOL WT : 273.42
------------- SUMMARY (AOP v1.91): HYDROXYL RADICALS -----------------
Hydrogen Abstraction       =  32.5985 E-12 cm3/molecule-sec
Reaction with N, S and -OH =  15.2800 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  47.8785 E-12 cm3/molecule-sec
   HALF-LIFE =     0.223 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =     2.681 Hrs
-------------- SUMMARY (AOP v1.91): OZONE REACTION -------------------

               ******  NO OZONE REACTION ESTIMATION ******
               (ONLY Olefins and Acetylenes are Estimated)
```

Experimental Database: NO Structure Matches

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; AOPWIN Program, Version 1.91; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: July 6, 2004
Order number for sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	Octadecanamide, N,N'-1,2-ethanediylbis- (CAS RN 110-30-5; Octadecanamide, N,N'-ethylenebis)
Purity:	Not applicable

Method

Method/guideline followed:	EPIWIN (v 3.11), AOPWIN Program (v 1.91)
Type:	Not applicable
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Concentration of substance:	Not applicable
Temperature (°C):	Not stated
Direct photolysis:	Not stated
Indirect photolysis:	Not stated
Breakdown products:	Not applicable
Remarks:	Overall OH Rate Constant: (k_{phot}) = 70 E-12 cm^3/molecule-sec; Half-life: $t_{1/2}$ = 1.8 hrs

Following are the results from the model:

```
AOP Program (v1.91) Results:
============================
SMILES : O=C(NCCNC(=O)CCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCC
CHEM   : Octadecanamide, N,N'-1,2-ethanediylbis-
MOL FOR: C38 H76 N2 O2
MOL WT : 593.04
------------- SUMMARY (AOP v1.91): HYDROXYL RADICALS --------------
Hydrogen Abstraction       =  59.4758 E-12 cm3/molecule-sec
Reaction with N, S and -OH =  11.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  70.4758 E-12 cm3/molecule-sec
   HALF-LIFE =     0.152 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =     1.821 Hrs
------------- SUMMARY (AOP v1.91): OZONE REACTION -----------------

              ******  NO OZONE REACTION ESTIMATION ******
              (ONLY Olefins and Acetylenes are Estimated)
```

```
Experimental Database:  NO Structure Matches
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; model data

References U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; AOPWIN Program, Version 1.91; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: July 6, 2004
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	Octadecanamide (CAS RN 124-26-5; Stearamide)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) Level III Fugacity Model; adapted from Mackay's EQC Level III Fugacity Model Media: Water, air, soil and sediment (model run with 1000 kg/hr emissions to water and 0 kg/hr emissions to air, soil and sediment)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 109 °C and boiling point of 250 °C.

Results

Remarks: Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Octadecanamide
  Molecular Wt: 283.5
  Henry's LC  : 1.04e-006 atm-m3/mole (Henrywin program)
  Vapor Press : 0.00398 mm Hg  (Mpbpwin program)
  Liquid VP   : 0.027 mm Hg  (super-cooled)
  Melting Pt  : 109 deg C (user-entered)
  Log Kow     : 6.7  (Kowwin program)
  Soil Koc    : 2.05e+006  (calc by model)

           Mass Amount    Half-Life    Emissions
            (percent)       (hr)       (kg/hr)
   Air       0.000363       9.5          0
   Water     12.8           360          1000
   Soil      0.00044        360          0
   Sediment  87.2           1.44e+003    0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       3.86e-015    0.327       0.0448      0.0327      0.00448
   Water     6.67e-013    303         158         30.3        15.8
   Soil      2.24e-020    0.0104      0           0.00104     0
   Sediment  2e-013       517         21.5        51.7        2.15


   Persistence Time: 1.23e+003 hr
```

```
Reaction Time:    1.5e+003 hr
Advection Time:   6.88e+003 hr
Percent Reacted:  82.1
Percent Advected: 17.9

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      9.497
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 2.817  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions:

Mass Amounts:
Air < 1 %
Water = 13 %
Soil < 1%
Sediment = 87 %

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: June 25, 2004
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	9-Octadecenamide, (Z)- (CAS RN 301-02-0; Oleamide)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) Level III Fugacity Model; adapted from Mackay's EQC Level III Fugacity Model Media: Water, air, soil and sediment (model run with 1000 kg/hr emissions to water and 0 kg/hr emissions to air, soil and sediment)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 76 °C.

Results

Remarks:	Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : 9-Octadecenamide, (Z)-
  Molecular Wt: 281.49
  Henry's LC  : 9.16e-007 atm-m3/mole (Henrywin program)
  Vapor Press : 1.2e-006 mm Hg  (Mpbpwin program)
  Liquid VP   : 3.83e-006 mm Hg  (super-cooled)
  Melting Pt  : 76 deg C (user-entered)
  Log Kow     : 6.48  (Kowwin program)
  Soil Koc    : 1.24e+006  (calc by model)

            Mass Amount    Half-Life    Emissions
             (percent)        (hr)       (kg/hr)
   Air       7.97e-005       1.27         0
   Water     14.4            360          1000
   Soil      0.000301        360          0
   Sediment  85.6            1.44e+003    0

              Fugacity    Reaction    Advection   Reaction    Advection
               (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       6.58e-016    0.509       0.00936     0.0509      0.000936
   Water     9.17e-013    326         170         32.6        17
   Soil      2.15e-020    0.00681     0           0.000681    0
   Sediment  2.75e-013    483         20.1        48.3        2.01

   Persistence Time: 1.17e+003 hr
   Reaction Time:    1.45e+003 hr
   Advection Time:   6.19e+003 hr
   Percent Reacted:  81
```

```
Percent Advected: 19

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      1.275
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 2.821  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions:

Mass Amounts:
Air < 1 %
Water = 14 %
Soil < 1%
Sediment = 86 %

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: June 25, 2004
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	13-Docosenamide, (Z)- (CAS RN 112-84-5; Erucamide)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) Level III Fugacity Model; adapted from Mackay's EQC Level III Fugacity Model Media: Water, air, soil and sediment (model run with 1000 kg/hr emissions to water and 0 kg/hr emissions to air, soil and sediment)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Remarks:	Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : 13-Docosenamide, (Z)-
  Molecular Wt: 337.59
  Henry's LC  : 2.84e-006 atm-m3/mole (Henrywin program)
  Vapor Press : 8.28e-008 mm Hg  (Mpbpwin program)
  Liquid VP   : 3.05e-006 mm Hg  (super-cooled)
  Melting Pt  : 183 deg C (Mpbpwin program)
  Log Kow     : 8.44  (Kowwin program)
  Soil Koc    : 1.13e+008  (calc by model)

            Mass Amount    Half-Life    Emissions
             (percent)        (hr)       (kg/hr)
   Air       1.3e-006        1.24         0
   Water     4.81            900          1000
   Soil      1.15e-005       900          0
   Sediment  95.2            3.6e+003     0

              Fugacity    Reaction    Advection   Reaction    Advection
               (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       2.53e-017    0.0253      0.000453    0.00253     4.53e-005
   Water     3.82e-014    129         167         12.9        16.7
   Soil      6.92e-023    0.000309    0           3.09e-005   0
   Sediment  2.57e-014    637         66.2        63.7        6.62



   Persistence Time: 3.48e+003 hr
   Reaction Time:    4.54e+003 hr
```

```
Advection Time:   1.49e+004 hr
Percent Reacted:  76.6
Percent Advected: 23.4

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      1.24
   Water:    900
   Soil:     900
   Sediment: 3600
     Biowin estimate: 2.697  (weeks-months)

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions:

Mass Amounts:
Air < 1 %
Water = 5 %
Soil < 1%
Sediment = 95 %

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: June 25, 2004
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	Dodecanamide, N-(2-hydroxyethyl)- (CAS RN 142-78-9)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) Level III Fugacity Model; adapted from Mackay's EQC Level III Fugacity Model Media: Water, air, soil and sediment (model run with 1000 kg/hr emissions to water and 0 kg/hr emissions to air, soil and sediment)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Remarks:	Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Dodecanamide, N-(2-hydroxyethyl)-
  Molecular Wt: 243.39
  Henry's LC  : 2.03e-011 atm-m3/mole (Henrywin program)
  Vapor Press : 6.57e-009 mm Hg  (Mpbpwin program)
  Liquid VP   : 1.24e-007 mm Hg  (super-cooled)
  Melting Pt  : 154 deg C (Mpbpwin program)
  Log Kow     : 3.24  (Kowwin program)
  Soil Koc    : 712  (calc by model)

            Mass Amount    Half-Life    Emissions
             (percent)        (hr)       (kg/hr)
   Air       1.39e-009       8.3          0
   Water     98.5            360          1000
   Soil      9.42e-006       360          0
   Sediment  1.55            1.44e+003    0

              Fugacity    Reaction    Advection   Reaction    Advection
               (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       5.85e-022    4.01e-007   4.8e-008    4.01e-008   4.8e-009
   Water     1.42e-016    656         341         65.6        34.1
   Soil      8.69e-024    6.28e-005   0           6.28e-006   0
   Sediment  6.17e-017    2.58        0.107       0.258       0.0107
```

```
Persistence Time: 346 hr
Reaction Time:    526 hr
Advection Time:   1.02e+003 hr
Percent Reacted:  65.9
Percent Advected: 34.1

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      8.302
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 3.065  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions:

Mass Amounts:
Air < 1 %
Water = 98 %
Soil < 1%
Sediment = 1 %

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: July 6, 2004
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	Dodecanamide, N,N-bis(2-hydroxyethyl)- (CAS RN 120-40-1)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) Level III Fugacity Model; adapted from Mackay's EQC Level III Fugacity Model Media: Water, air, soil and sediment (model run with 1000 kg/hr emissions to water and 0 kg/hr emissions to air, soil and sediment)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 38.7 °C.

Results

Remarks: Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Dodecanamide, N,N-bis(2-hydroxyethyl)-
  Molecular Wt: 287.45
  Henry's LC  : 2.16e-012 atm-m3/mole (Henrywin program)
  Vapor Press : 6.73e-009 mm Hg  (Mpbpwin program)
  Liquid VP   : 9.19e-009 mm Hg  (super-cooled)
  Melting Pt  : 38.7 deg C (user-entered)
  Log Kow     : 2.89  (Kowwin program)
  Soil Koc    : 318  (calc by model)

           Mass Amount    Half-Life    Emissions
            (percent)       (hr)       (kg/hr)
   Air       1.89e-010      5.21         0
   Water     99.1           360          1000
   Soil      9.95e-007      360          0
   Sediment  0.905          1.44e+003    0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       5.58e-024    8.64e-008   6.49e-009   8.64e-009   6.49e-010
   Water     1.28e-017    657         341         65.7        34.1
   Soil      1.8e-025     6.59e-006   0           6.59e-007   0
   Sediment  6.78e-018    1.5         0.0624      0.15        0.00624

   Persistence Time: 344 hr
   Reaction Time:    523 hr
   Advection Time:   1.01e+003 hr
```

```
Percent Reacted:  65.9
Percent Advected: 34.1

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      5.208
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 3.128  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions:

Mass Amounts:
Air < 1 %
Water = 99 %
Soil < 1 %
Sediment < 1 %

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: July 6, 2004
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)- (CAS RN 93-83-4, Oleamide, N,N-bis(2-hydroxyethyl)-)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) Level III Fugacity Model; adapted from Mackay's EQC Level III Fugacity Model Media: Water, air, soil and sediment (model run with 1000 kg/hr emissions to water and 0 kg/hr emissions to air, soil and sediment)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Remarks:	Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : 9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)-
  Molecular Wt: 369.59
  Henry's LC  : 1.04e-011 atm-m3/mole (Henrywin program)
  Vapor Press : 5.88e-013 mm Hg  (Mpbpwin program)
  Liquid VP   : 3.43e-011 mm Hg  (super-cooled)
  Melting Pt  : 204 deg C (Mpbpwin program)
  Log Kow     : 5.62  (Kowwin program)
  Soil Koc    : 1.71e+005  (calc by model)

           Mass Amount    Half-Life    Emissions
            (percent)       (hr)       (kg/hr)
   Air       4.21e-009      1.11         0
   Water     34.1           360          1000
   Soil      7.66e-008      360          0
   Sediment  65.9           1.44e+003    0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       7.97e-025    1.99e-005   3.17e-007   1.99e-006   3.17e-008
   Water     2.83e-017    495         257         49.5        25.7
   Soil      2.2e-028     1.11e-006   0           1.11e-007   0
   Sediment  8.5e-018     239         9.92        23.9        0.992

   Persistence Time: 753 hr
   Reaction Time:    1.03e+003 hr
   Advection Time:   2.82e+003 hr
   Percent Reacted:  73.3
```

```
Percent Advected: 26.7

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      1.106
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 2.946  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions:

Mass Amounts:
Air < 1 %
Water = 34 %
Soil < 1%
Sediment = 66 %

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: July 6, 2004
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	Amides, C12-18, N,N-bis(hydroxyethyl) (CAS RN 68155-06-6)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) Level III Fugacity Model; adapted from Mackay's EQC Level III Fugacity Model Media: Water, air, soil and sediment (model run with 1000 kg/hr emissions to water and 0 kg/hr emissions to air, soil and sediment)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Remarks:	Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Amides, C12-18, N,N-bis(hydroxyethyl)
  Molecular Wt: 273.42
  Henry's LC  : 1.63e-012 atm-m3/mole (Henrywin program)
  Vapor Press : 9.91e-010 mm Hg  (Mpbpwin program)
  Liquid VP   : 1.86e-008 mm Hg  (super-cooled)
  Melting Pt  : 154 deg C (Mpbpwin program)
  Log Kow     : 2.39  (Kowwin program)
  Soil Koc    : 101  (calc by model)

           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       5.45e-011       5.36         0
   Water     99.5            360          1000
   Soil      7.37e-007       360          0
   Sediment  0.459           1.44e+003    0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       3.38e-024    2.42e-008   1.87e-009   2.42e-009   1.87e-010
   Water     1.02e-017    658         342         65.8        34.2
   Soil      3.09e-025    4.87e-006   0           4.87e-007   0
   Sediment  6.88e-018    0.758       0.0315      0.0758      0.00315

   Persistence Time: 343 hr
   Reaction Time:    521 hr
   Advection Time:   1e+003 hr
   Percent Reacted:  65.8
```

```
Percent Advected: 34.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      5.362
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 3.159  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions:

Mass Amounts:
Air < 1 %
Water = 99 %
Soil < 1%
Sediment = 0.5 %

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: July 6, 2004
Order number for sorting:
Remarks:

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	Octadecanamide, N,N'-1,2-ethanediylbis- (CAS RN 110-30-5; Octadecanamide, N,N'-ethylenebis)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) Level III Fugacity Model; adapted from Mackay's EQC Level III Fugacity Model Media: Water, air, soil and sediment (model run with 1000 kg/hr emissions to water and 0 kg/hr emissions to air, soil and sediment)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Remarks:	Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Octadecanamide, N,N'-1,2-ethanediylbis-
  Molecular Wt: 593.04
  Henry's LC  : 1.49e-007 atm-m3/mole (Henrywin program)
  Vapor Press : 7.97e-018 mm Hg  (Mpbpwin program)
  Liquid VP   : 7.02e-015 mm Hg  (super-cooled)
  Melting Pt  : 323 deg C (Mpbpwin program)
  Log Kow     : 14  (Kowwin program)
  Soil Koc    : 3.92e+013  (calc by model)

           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       4.99e-013       3.64         0
   Water     4.79            900          1000
   Soil      1.75e-011       900          0
   Sediment  95.2            3.6e+003     0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       5.58e-032    3.31e-009   1.74e-010   3.31e-010   1.74e-011
   Water     3.3e-021     128         167         12.8        16.7
   Soil      9.05e-036    4.69e-010   0           4.69e-011   0
   Sediment  2.22e-021    638         66.3        63.8        6.63

   Persistence Time: 3.48e+003 hr
   Reaction Time:    4.54e+003 hr
   Advection Time:   1.49e+004 hr
   Percent Reacted:  76.7
```

```
Percent Advected: 23.3

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      3.643
   Water:    900
   Soil:     900
   Sediment: 3600
     Biowin estimate: 2.377  (weeks-months)

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions:

Mass Amounts:
Air < 1 %
Water = 5 %
Soil < 1%
Sediment = 95 %

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed: July 6, 2004
Order number for sorting:
Remarks:

3.5 BIODEGRADATION

Test Substance

Identity: Oleylamide (CAS RN 301-02-0; Oleamide)
Purity: 97%
Remarks:

Method

Method/Guideline followed: OECD Guideline 301D, EEC Method C.6. and ISO/TC 147/SC 5WG 4N152
Test type: Aerobic ready biodegradability
GLP: Yes
Year: 1993
Contact time: 28 days
Inoculum: Activated sludge
Remarks: The test substance was measured for ready biodegradability in a closed bottle system. BOD bottles (250 - 300 ml) were prepared to contain a mineral nutrient solution together with the following treatments: inoculum only, test substance with inoculum, and sodium acetate (used as a reference substance) with inoculum. The concentrations of the test substance and sodium acetate were 2.0 and 6.7 mg/l, which represented theoretical oxygen demands of 2.9 mg/mg and 0.8 mg/mg, respectively. Ten replicate bottles were prepared for each experimental group and incubated at 21±1 °C. At 0, 7, 14, 21 and 28 days, two bottles from each treatment were measured for dissolved oxygen concentrations. The pH of the medium was 7.1 at the start of the test and 6.6 – 6.7 at day 28. Temperature ranged from 20 to 22 °C.

Results

Degradation: 80% degradation in 28 days
Results: The results indicate that the test substance was readily biodegradable under the conditions of the test.
Kinetic: % Degradation

Day	Test Substance	Reference Substance
7	62	16
14	69	85
21	76	81
28	80	82

Breakdown products: Not stated

Remarks:	The validity of the test was demonstrated by an endogenous respiration of 0.9 mg/l at day 28, differences of the replicate values of the control at day 28 were less than 20%, the reference material was degraded to 85% by day 14, and oxygen consumption in all bottles was > 0.5 mg/l during the test period.

Conclusions

Remarks:	The test material was readily biodegradable. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

van Ginkel, C. G. and C. A. Stroo. 1993. Biodegradability of Armid O Pastilles in the Closed Bottle Test. Report number CRL F93009. Akzo Research Laboratories, Arnhem, The Netherlands.

Other Available Reports

Other

Last changed:	July 20, 2000
Order number for sorting:	75
Remarks:	

3.5 BIODEGRADATION

Test Substance

Identity:	Erucamide (CAS RN 112-84-5)
Purity:	97.5%
Remarks:	

Method

Method/Guideline followed:	Methods conformed to OECD Guideline 301D and EEC Method C.6
Test type:	Aerobic ready biodegradability
GLP:	Yes
Year:	1993
Contact time:	140 days
Inoculum:	Secondary activated sludge
Remarks:	The study assessed the aerobic biodegradation of the test substance in a closed bottle system. Activated sludge was preconditioned in the laboratory by aeration for a period of one week to reduce endogenous respiration. Ten replicate BOD bottles were prepared for each of three treatment groups. Treatment groups included a blank control, test substance at 2.0 mg/l, and reference substance (sodium acetate) at 6.7 mg/l. All test solutions were made in nutrient medium and contained activated sludge inoculum at 2 mg dry weight/l. After the BOD bottles were prepared, they were incubated in the dark at 20 to 22 °C. On days 0, 7, 14, and 21, two BOD bottles from each group were destructively sampled for dissolved oxygen concentrations. Oxygen measurements made on day 28 used a device that replaced the test solutions. The test was extended and additional dissolved oxygen measurements were made on days 42, 56, 84, 112 and 140. Percent biodegradation was calculated as the quotient of the measured biological oxygen demand to the theoretical oxygen demand. The theoretical oxygen demand of the test substance was the mg O_2/mg test substance based on the molecular formula that could be used in bacterial respiration. A substance is considered to be readily biodegradable if the percent biodegradation is ≥60% at 28 days.

Results

Degradation:	Biodegradation of the test substance was 15% at day 28 and 43% at day 140
Results:	The results indicate that the test substance was not readily biodegradable but can be considered inherently biodegradable under the conditions of the test.

Kinetic: % Degradation

Day	Test Substance	Reference Substance
7	8	76
14	10	85
21	7	81
28	15	82
42	23	
56	26	
84	34	
112	41	
140	43	

Breakdown products: Not stated
Remarks: The validity of the test was demonstrated by biodegradation of the reference substance, an endogenous respiration of 0.9 mg/l at day 28, and difference between replicate values of < 20%.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1A
Remarks: Reliable without restriction; guideline study.

References

van Ginkel, C. G. and C. A. Stroo. 1993. Biodegradability of Armid E in the Closed Bottle Test. Report number CRL F93035. Akzo Research Laboratories, Arnhem, The Netherlands.

Other Available Reports

Other

Last changed: July 20, 2000
Order number for sorting: 32
Remarks:

3.5 BIODEGRADATION

Test Substance

Identity:	Erucamide (CAS RN 112-84-5)
Purity:	> 97% total amide content
Remarks:	

Method

Method/Guideline followed:	Methods conformed to OECD Guideline 301B and EEC Method C.5
Test type:	Aerobic ready biodegradability
GLP:	Yes
Year:	1991
Contact time:	28 days
Inoculum:	Activated sludge
Remarks:	Freshly-collected activated sludge was aerated for 4 hours, then left to settle for ½hour. The supernatant was decanted to provide sufficient volume to prepare a 1% inoculum for each test flask. Test vessels were 3-l brown glass bottles. Initially, 30 ml of inoculum was added to an amount of mineral nutrient solution in each of four test vessels. The solutions were aerated with CO_2-free air for 24 hours. After the aeration period, three CO_2-absorber bottles filled with 80 ml 0.025N $Ba(OH)_2$ were connected to the exit line of each bottle. The test substance was added to two bottles, a reference material (sodium acetate) was added to a third bottle, while the fourth bottle contained only inoculum and nutrient solution. All vessels were brought to a volume of 3 l with purified water (Milli-Q®). Final concentrations of the test substance were 10 and 20 mg/l. The concentration of sodium acetate was 20 mg/l. Because the solubility of the test substance in water was low, it was quantitatively added to the test media and continuously stirred during the test. The CO_2 produced by the degradation of the test substance by the inoculum was subsequently trapped in the $Ba(OH)_2$ solution. The amount of CO_2 produced was determined by titrating the $Ba(OH)_2$ with HCl. Biodegradation was calculated as the amount of CO_2 produced divided by the amount of CO_2 that could theoretically have been produced based on the amount of carbon (as test substance) added to the test vessels. The target temperature for the test was 18 - 22 °C. During the test, the temperature of the test room varied between 18 and 21.5 °C with one incidental extreme of 23 °C.

Results

Degradation: The results indicate that the test substance was not readily biodegradable but can be considered inherently biodegradable under the conditions of the test.

Results: Biodegradation achieved 27 and 15% in the 10 and 20 mg/l test substance concentrations, respectively.

Kinetic: % Degradation

Day	Test Substance 10 mg/L	Test Substance 20 mg/L
2	0	0
5	0.7	0.3
7	2.6	0.6
9	4.2	1.3
12	4.2	1.4
16	8.8	6.2
21	16.4	11.3
28	27.2	15.2

Breakdown products: Not stated

Remarks: The test was considered acceptable based upon biodegradation of the reference substance of 60% within 20 days and 71% by the end of 28 days.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1A

Remarks: Reliable without restriction; guideline study.

References

Coenen, T. M. M. and H. Berkhout. 1991. Ready Biodegradability: Modified Sturm Test with UNISLIP ERUCAMIDE. Report number 052572. RCC NOTOX B. V., 's-Hertogenbosch, The Netherlands.

Other Available Reports

Other

Last changed: July 20, 2000

Order number for sorting: 33

Remarks:

3.5 BIODEGRADATION

Test Substance

Identity:	Tallowamide (hydrogenated tallow-alkyl) (CAS RN 61790-31-6; Amides, tallow, hydrogenated)
Purity:	97.0%
Remarks:	

Method

Method/Guideline followed:	Methods conformed to OECD 301D and EEC Method C.6.
Test type:	Aerobic ready biodegradability
GLP:	Yes
Year:	1993
Contact time:	28 days
Inoculum:	Secondary activated sludge
Remarks:	The study assessed the aerobic biodegradation of the test substance in a closed bottle system. Activated sludge was preconditioned in the laboratory by aeration for a period of one week to reduce endogenous respiration. Ten replicate BOD bottles were prepared for each of three treatment groups. Treatment groups included a blank control (nutrient medium with inoculum), test substance at 2.0 mg/l, and reference substance (sodium acetate) at 6.7 mg/l). All test solutions were made in nutrient medium and contained activated sludge inoculum at 2 mg dry weight/l. After the BOD bottles were prepared, they were incubated in the dark at 20 to 22 °C. On days 0, 7, 14, 21, and 28, two BOD bottles from each group were destructively sampled for dissolved oxygen concentrations. The pH of the medium was 7.0 at the start and 6.7 at day 28. Temperature ranged from 20 to 22 °C. Percent biodegradation was calculated as the quotient of the measured biological oxygen demand to the theoretical oxygen demand. The theoretical oxygen demand of the test substance was the mg O_2/mg test substance based on the molecular formula that could be used in bacterial respiration. A substance is considered to be readily biodegradable if the percent biodegradation is ≥60%.

Results

Degradation:	The test substance was biodegraded 73% at day 28
Results:	The amount of biodegradation indicated that the test substance was readily biodegradable under the conditions of the test.

Kinetic: % Degradation

Day	Test Substance	Reference Substance
7	50	76
14	59	85
21	72	81
28	73	82

Breakdown products: Not stated
Remarks: The validity of the test was demonstrated by biodegradation of the reference substance, an endogenous respiration of 0.9 mg/l at day 28, difference between replicate values in the control group at day 28 was < 20%, and oxygen concentrations > 0.5 mg/l in all bottles during the test period.

Conclusions

Remarks: The test substance was readily biodegradable.
The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 1A
Remarks: Reliable without restriction; guideline study.

References

van Ginkel, C. G. and C. A. Stroo. 1993. Biodegradability of Armid HT Flakes in the Closed Bottle Test. Report number CRL F93008. Akzo Research Laboratories, Arnhem, The Netherlands.

Other Available Reports

Other

Last changed: July 20, 2000
Order number for sorting: 158
Remarks:

3.5 BIODEGRADATION

Test Substance

Identity:	Dodecanamide, N,N-bis(2-hydroxyethyl)- (CAS RN 120-40-1)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Method based on the CO_2 production test described by Sturm, R. N. 1973. Biodegradability of Nonionic Surfactants: Screening Test for Prediction Rate and Ultimate Biodegradation. J. Am. Oil Chemists Soc. 50(5):159 - 167.
Test type:	Aerobic ultimate biodegradability
GLP:	No
Year:	1974
Contact time:	40 days
Inoculum:	Acclimated raw sewage microorganisms
Remarks:	Preceding the test, microorganisms contained in raw sewage are acclimated for 14 days to the specific test substance. At the end of the acclimation period, the acclimated sewage seed was used to inoculate the test carboys. Concentrations of the test substance (20 mg/L), a reference material, dextrose (20 mg/L), and blanks (carboys without test substance or reference material) were prepared in a mineral nutrient solution and inoculated with a volume of the acclimated sewage seed. The carboys were aerated with CO_2-free air and the effluent air passes through a series of $Ba(OH)_2$ traps, which collect any evolved CO_2. Periodically, the trap closest to the carboy was removed and titrated with HCl to determine the amount of CO_2 collected in the trap. This continued for 40 days. The percent biodegradation was calculated as the amount of CO_2 collected in the traps divided by the amount of CO_2 that could possibly be evolved based on the chemical formula of the test substance.

Results

Results:	Biodegradation achieved 77% by 28 days and 79.7% by the end of the test.

Kinetic: % Degradation

Day	Test Substance
2	9
3	20
4	30
6	42
7	55
10	64
14	75
18	77
28	77
40	79.7

Breakdown products: Not stated
Remarks: The reference substance attained 77.5% degradation in 18 days.

Conclusions

Remarks: The test material showed ultimate biodegradation (>70%) under the conditions of the study..
The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2B
Remarks: Reliable with restrictions; basic data given, comparable to guidelines/standards.

References

Bishop, W. E. 1974. Ultimate Biodegradability Via CO_2 Production with Cover Letter Dated 5/123/96. EPA document number 86960000530. Proctor and Gamble Co., Cincinnati, OH, U. S.

Other Available Reports

Other

Last changed: July 20, 2000
Order number for sorting: 43
Remarks:

3.5 BIODEGRADATION

Test Substance

Identity:	Amides, coco, N,N-bis(hydroxyethyl) (CAS RN 68603-42-9)
Purity:	100%
Remarks:	

Method

Method/Guideline followed:	Methods conformed to Modified Closed Bottle Method, U. S. EPA TSCA 40 CFR 796, Guideline 796.3200
Test type:	Aerobic ready biodegradability
GLP:	No, but the report incorporated many GLP requirements
Year:	1986
Contact time:	28 days
Inoculum:	Composite of settled activated sludge and garden soil. Two liters of activated sludge were allowed to settle for 45 minutes, and supernatant was collected for use. One hundred grams of garden soil was added to 1 l of deionized water, mixed and allowed to settle for 30 minutes, and supernatant was collected for use. One hundred milliliters of each fraction was combined and aerated until use.
Remarks:	The study assessed the aerobic biodegradation of the test substance in a closed bottle system. Duplicate BOD bottles were used for each experimental group. Treatment groups consisted of a blank control, the test substance at 3 mg active/l and a reference compound (sodium benzoate) at 3 mg active/l. Test solutions were made with nutrient mineral solution. After filling the BOD bottles, they were placed in a BOD incubator at 20±1 °C. After 5, 15, 21 and 28 days, the dissolved oxygen concentration in each bottle was measured using a dissolved oxygen probe. Liquid lost during measuring was replaced with oxygen-free water. Percent biodegradation was calculated as the quotient of the measured biological oxygen demand to the theoretical oxygen demand. The theoretical oxygen demand of the test substance was the mg O_2/mg test substance based on the molecular formula that could be used in bacterial respiration. The test substance was considered to be readily biodegradable if the percent biodegradation was ≥ 60%.

Results

Degradation:	The average percent biodegradation of the test substance was 51.8% in 28 days.

Results: The results indicate that the test substance was not readily biodegradable but can be considered inherently biodegradable under the conditions of the test.

Kinetic: % Degradation

Day	Test Substance	Reference Substance
5	30	75
15	55	99
21	59	109
28	52	94

Not stated

Breakdown products: Not stated

Remarks: The validity of the test was confirmed by a percent biodegradation of ≥ 60% in the reference compound, sodium benzoate.

Conclusions

Remarks: The test material was inherently biodegradable.
The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1B

Remarks: Reliable without restriction; comparable to guideline study.

References

Pence, W. H. 1986. The Evaluation of the Biodegradation Potential of Test Materials Using a Modified Closed Bottle Method. Report number 86-0836-11. Hill Top Research, Inc., Cincinnati, OH, U. S.

Other Available Reports

Other

Last changed: July 24, 2000

Order number for sorting: 136

Remarks:

3.5 BIODEGRADATION

Test Substance

Identity:	Amides, coco, N-(hydroxyethyl) (CAS RN 68140-00-1)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Methods conformed to Coupled Units Test (Model Sewage Treatment Plant); corresponding to OECD Guideline 303A
Test type:	Aerobic ready biodegradability
GLP:	Not stated
Year:	1998
Contact time:	Not stated
Inoculum:	Activated sludge
Remarks:	Two OECD confirmatory test units were operated in parallel whereby the parallelism was enhanced and assured by a transinoculation procedure. The test material (10 mg dissolved organic carbon (DOC)/l) was added to the influent of one unit while the other was fed synthetic sewage. The DOC concentrations were measured in both effluents.

Results

Degradation:	At a test concentration of 10 mg carbon/l and a hydraulic retention time of 3 hours, the carbon elimination rate (DOC removal) was 92 ± 6%
Results:	The data demonstrated that the test substance could be regarded as easily biodegradable under the condition of the biological sewage treatment plant (author of the report).
Kinetic:	Not stated
Breakdown products:	Not stated
Remarks:	

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Basic data given, No study details were available; comparable to guidelines/standards.

References

H. Berger and Guhl. 1998. Biological Research and Product Safety/Ecology: Unpublished Results, Test substance registration number 7811. Henkel KGaA, Duesseldorf, Germany.

Other Available Reports

Other

Last changed: July 20, 2000
Order number for sorting: 113
Remarks:

3.5 BIODEGRADATION

Test Substance

Identity: Amides, C12-18, N,N-bis(hydroxyethyl (CAS RN 68155-06-6)
Purity: Not stated
Remarks:

Method

Method/Guideline followed: OECD Guideline 301D (also EEC-Directive 92/69/EEC Annex V, Part C, EEC C.4. and C.4 - E)
Test type: Closed bottle test
GLP: Not stated
Year: 1996
Contact time: 28 days
Inoculum: Effluent
Remarks: The solution of the test substance in mineral medium, usually at 2 or 5 mg/l, was inoculated with a relatively small number of micro-organisms from the effluent of a municipal sewage treatment plant and kept in completely filled, closed bottles in the dark at constant temperature (20°C). Degradation was followed by analysis of dissolved oxygen over a 28-day period. The BOD, i.e. the amount of oxygen consumed by the microbial population during biodegradation of the test substance, corrected for oxygen uptake by the blank inoculum run in parallel, was expressed as a percentage of ThOD or COD.

Results

Degradation: 84% degradation in 28 days at 2 mg/l active matter and 71% degradation in 28 days at 5 mg/l active matter.
Results: Based on the data received the test substance meets the OECD criteria for "ready biodegradability" (> 60% BOD/COD or BOD/ThOD within a 10 day "time window").
Kinetic: % Degradation

Day	Test Substance	Reference Substance
7	21	22
14	70	54
21	70	65
28	84	71

Breakdown products: Not stated
Remarks:

Conclusions

Remarks:	The test material was readily biodegradable. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Basic data given, No study details were available; comparable to guidelines/standards.

References

Steber, J. and H. Berger. 1996. Biological Research and Product Safety/Ecology. Report number R9501453. Henkel KGaA, Duesseldorf, Germany.

Steber, J. and H. Berger. Biological Research and Product Safety/Ecology: Unpublished results; test substance registration number SAT 950975. Henkel KGaA, Duesseldorf, Germany.

Other Available Reports

Other

Last changed:	August 1, 2000
Order number for sorting:	131
Remarks:	

3.5 BIODEGRADATION

Test Substance

Identity:	*Sanitized report: chemical name not specified.* (CAS RN 68910-93-0; Fatty acids, tall-oil, reaction products with polyethylenepolyamines)
Purity:	Monoalkylamide ≅ 80% Dialkylamide ≅ 20% Free DEP ≅ 1.3% Water ≅ 0.5%
Remarks:	In addition to the CAS number, the following was given as the chemical name: "Reaction product of tall oil fatty acid and aminoethylpiperazine".

Method

Method/Guideline followed:	OECD Guideline 301D and EEC Methods 4.1 and 4.2
Test type:	Aerobic ready biodegradability
GLP:	Yes
Year:	1990
Contact time:	126 days
Inoculum:	Secondary activated sludge
Remarks:	The test substance was measured for ready biodegradability in a closed bottle test system. BOD bottles (280 ml) were prepared to contain a mineral nutrient solution together with the following treatments: mineral solution without inoculum, mineral solution with inoculum, mineral solution with test substance and inoculum, and mineral solution with sodium acetate (used as a reference substance) with inoculum. The concentrations of the test substance and sodium acetate were 2.0 and 6.7 mg/l, which represented theoretical oxygen demands of 2.9 g O_2/g test substance and 0.8 g O_2/g reference substance, respectively. The amount of biodegradation was calculated as the ratio of the biochemical oxygen demand (BOD) to the theoretical oxygen demand (ThOD). Vessels containing the test substance were measured periodically for dissolved oxygen concentrations.

Results

Degradation:	Partly degraded (30 – 40%) in the test.
Results:	The results indicate that the test substance was not readily biodegradable but can be considered inherently biodegradable under the conditions of the test

Kinetic: % Degradation

Day	Test Substance	Reference Substance
5	12	69
15	33	83
28	36	90
42	38	
70	36	
98	34	
126	34	

Breakdown products: Not stated

Remarks: There was no significant degradation after day 15. The partial biodegradation indicates the formation of a recalcitrant intermediate, although the test substance or the intermediate may not be recalcitrant in nature. The lack of biodegradation was not due to toxicity of the test compound because endogenous respiration was not inhibited. The validity of the test was demonstrated by an endogenous respiration of 0.4 mg/l at day 28, the reference material was degraded to 90% by day 28, and the pH of the medium was 7.5 on day 28.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1A

Remarks: Reliable without restriction; guideline study.

References

van Ginkel, C. G. 1990. Biodegradability of [CAS RN 68910-93-0]. Report number T 90-02-01.9. Akzo Research Laboratories, Arnhem, The Netherlands.

Other Available Reports

Other

Last changed: July 24, 2000

Order number for sorting: 149

Remarks:

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Erucamide (CAS RN 112-84-5)
Purity:	100% commercial product (99% total amide)
Remarks:	Complete characterization provided in report

Method

Method/Guideline followed:	ISO/DIS 10229-1 and Crossland, N. O., 1986, Chemosphere, 14:1855
Type:	Flow-through
GLP:	Yes
Year:	1994
Species/Strain/Supplier:	Zebra fish (*Brachydanio rerio*)
Analytical monitoring:	Yes, GC/FID
Exposure period:	28 days
Statistical methods:	Analysis of Variance and Dunnett's Test (if required)
Remarks:	The experiment measured the growth and growth rate of juvenile fish after 14 and 28 days of exposure to the test and control substances. No significant mortalities occurred in the group of cultured fish the week prior to test initiation. The following four experimental groups were used in a flow-through exposure system: control (dilution water), solvent control (0.02 ml methanol/L), 32 µg/l, and 105 µg/l (nominal concentrations). Flow rates of the test solutions were a nominal 67 mL/minute giving approximately 10 volume replacements/day. Treatments were contained in single 12-liter glass vessels containing 10 liters of solution. Replicate test vessels were not used. Fish were fasted for 24 hours prior to test initiation at which time 16 fish were randomly transferred to the test vessels and the vessels were randomly placed in the test area. Test vessels were aerated during the test. Light intensity was not measured, but ambient laboratory lighting was provided with a photoperiod of 16 hours light/8 hours dark. Water pH, dissolved oxygen (DO), and temperature were measured in each test vessel daily except weekends. Total hardness (as $CaCO_3$) was measured in the control vessel daily except weekends. Means and ranges for temperature, pH, DO and total hardness were 23.1 °C (22.5 – 23.5 °C), 7.5 (7.1 – 7.8), 8.5 mg/l (7.7 – 10.2) and 100 mg/l (86 – 108 mg/l), respectively. The pH, DO, temperature and total hardness remained within acceptable limits during the test. Concentrations of the test substance in the exposure solutions were measured on test days - 1, 0, 3, 4, 11, 13, 18,

20, 25 and 27. Effect concentrations were based on mean measured concentrations.

Results

Nominal concentrations (µg/l):	0 (control), 0 (solvent control), 32 and 105
Measured concentrations (µg/l):	< 1.0, < 1.0, 31.8 and 105.3
Unit:	µg/l
Element value:	28-day NOEC = > 105.3 µg/l
Statistical results:	The NOEC was not defined as no inhibitory effects of the test substance were measured at the highest test concentration.
Remarks:	The NOEC was > 105.3 µg/l. A diluter malfunction occurred on test day 3 resulting in blockage of the dilution water flow into the 105 µg/l treatment and causing a rise in the concentration to 218 µg/l. Concurrently, the control vessel became contaminated with test substance to a concentration of 78 µg/l. By test day 4, concentrations in the control tank had fallen to 0.1 µg/l. The short exposure of the control fish to the test substance was not thought to have affected the test results. Concentrations of test solutions averaged 96 and 105% in the two treatment levels (range 56 – 160%).

Conclusions

Remarks:	The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Marshall, S. J. and S. R. Harding. 1994. The Chronic Toxicity of UNISLIP 1753 to *Brachydanio rerio* Under Continuous Flow Conditions: 28 Day Growth Test. Report number CT/N25/01. Unilever Research, Port Sunlight Laboratory, Merseyside, UK.

Other Available Reports

Other

Last changed:	July 20, 2000
Order number for sorting:	34
Remarks:	

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Amide, coco, N,N-bis(hydroxyethyl) (CAS RN 68603-42-9)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Methods conformed to EU Commission Directive 92/69/EEC, Method C.1, method corresponds to OECD Guideline 203
Type:	Static-renewal
GLP:	Not stated
Year:	1999
Species/Strain/Supplier:	Zebra fish (*Brachydanio rerio*)
Analytical monitoring:	Not stated
Exposure period:	96 hours
Statistical methods:	Not stated
Remarks:	The experiment measured the 96-hour acute toxicity of the test substance to Zebra fish in a static-renewal test system. Test solutions were renewed fresh every 24 hours. Ten fish were exposed to each treatment level. Mortalities were recorded at least every 24 hours. The following values were calculated: LC_0 = Highest concentration showing no mortality LC_{50} = Concentration showing 50% mortality LC_{100} = Lowest concentration in which all animals died.

Results

Nominal concentrations (mg/l):	Not stated
Measured concentrations (mg/l):	Not stated
Unit:	mg active matter/l
Element value:	96-hour LC_{50}
Statistical results:	96-hour LC_{50} = 6.7 mg active matter/l
Remarks:	Additional results calculated were: LC_0 = 5.6 mg active matter/l LC_{100} = 8.0 mg active matter/l

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Reliable with restrictions; basic data given, comparable to guidelines/standards.

References

Steber, J. and H. Berger. 1999. Biological Research and Product Safety/Ecology: Report number 1986/2497. Henkel KGaA, Duesseldorf, Germany.

Steber, J. and H. Berger. 1999. Biological Research and Product Safety/Ecology: unpublished results; Test substance registration number Fi 6650. Henkel KGaA, Duesseldorf, Germany.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	137
Remarks:	

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Oleamide, N,N-bis(2-hydroxyethyl)- (CAS RN 93-83-4)
Purity:	100%
Remarks:	

Method

Method/guideline followed:	Not stated
Type:	Static
GLP:	No
Year:	1992
Species/Strain/Supplier:	Fathead minnow (*Pimephales promelas*)/laboratory culture
Analytical monitoring:	No
Exposure period:	96 hours
Statistical methods:	LC_{50} values were calculated using either the Trimmed Spearman-Karber Method or the log-probit transformation
Remarks:	The experiment measured the acute toxicity of the test substance to Fathead minnows during a 96-hour exposure period. Treatment levels consisted of a dilution water control and 0.625, 1.25, 2.50, 5.00, and 10.0 mg/l of test substance. Twenty fish were exposed to each test level. Dilution water was dechlorinated Milwaukee tap water. Test vessels were glass aquaria holding 15 liters of test solution. Fish were fed twice daily prior to testing, but were not fed during the test. The photoperiod was 12 hours light/dark during fish acclimation and testing. After test initiation, fish were observed every 24 hours for mortalities. Dead fish were removed and weighed when observed. Surviving fish were weighed at the end of the test. Temperature and dissolved oxygen was measured in each test vessel every 24 hours. Water pH, total alkalinity and hardness were measured at the beginning and end of the test in each test solution. The following values represented conditions during the test: Mean fish weight = 0.183 g Mean temperature = 20.3 °C Mean dissolved oxygen = 8.74 mg/l Average pH = 8.4 Mean alkalinity = 115.8 mg $CaCO_3$/l Mean hardness = 164.4 mg $CaCO_3$/l.

Results

Nominal concentrations (mg/l):	0 (control), 0.625, 1.25, 2.50, 5.00, 10.0
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
Element value:	96-hour LC_{50}
Statistical results:	96-hour LC_{50} = 2.6 mg/l (95% confidence interval = 2.10 – 3.22 mg/l)
Remarks:	Additional LC_{50} values were determined to be: 24-hour LC_{50} = 7.1 mg/l (no confidence interval) 48-hour LC_{50} = 3.0 mg/l (2.29 – 3.94 mg/l) 72-hour LC_{50} = 2.6 mg/l (2.10 – 3.22 mg/l)

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Reliable with restrictions; basic data given, comparable to guideline standards.

References

Goodrich, M., K. Kosteretz and J. Lech. 1992. Supplemental Information: Letter submitting Toxicity of [CAS number 93-83-4] in Fathead Minnows (Final Report) (Sanitized). U. S. EPA document number 89-920000188S. NIEHS Aquatic Biomedical Core Center. University of Wisconsin, Milwaukee, WI, U. S.

Other Available Reports

Other

Last changed:	July 20, 2000
Order number for sorting:	2
Remarks:	

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	*Sanitized report: chemical name not specified.* (CAS RN 68910-93-0; Fatty acids, tall-oil, reaction products with polyethylenepolyamines)
Purity:	Monoalkylamide ≅ 80% Dialkylamide ≅ 20% Free DEP ≅ 1.3% Water ≅ 0.5%
Remarks:	In addition to the CAS number, the following was given as the chemical name: "Reaction product of tall oil fatty acid and aminoethylpiperazine".

Method

Method/Guideline followed:	EEC Method C.1 and OECD Guideline 203
Type:	Static-renewal
GLP:	Yes
Year:	1990
Species/Strain/Supplier:	*Brachydanio rerio* (Zebra fish)
Analytical monitoring:	No
Exposure period:	96 hours
Statistical methods:	LC_{50} calculated using an LC_{50} program of Griffioen (RIZA) based on a model of Kooyman (1981)
Remarks:	The experiment measured the acute toxicity of the test substance to fish over a 96-hour exposure period. Fresh test solutions were made at 48 hours. Five concentrations of the test substance and a control group were used in the test: 0 (control), 0.18, 0.32, 0.56, 1.0, and 1.8 mg/l. Seven fish were exposed to each treatment and control group. No replicates were used. Test vessels were 5-liter glass aquaria containing 3 liters of test medium. Vessels were covered with a glass plate during the test. Dilution water used in the test was synthetic water ("Dutch Standard Water") having a pH of approximately 8.2 and a hardness of 13°dH. The biomass loading during the test was approximately 0.7 g of biomass/l. The test medium was not aerated and the fish were not fed during the test. Test vessels were placed in a temperature controlled area between 21 and 25 °C. A photoperiod of 12 hours light/12 hours dark was provided by fluorescent lights. Measurements of pH and dissolved oxygen were made daily, and temperature was continuously measured in one test vessel. Dissolved oxygen ranged from 5.9 to 8.9 mg/l, pH ranged from 7.5 to 8.1 and temperature ranged from 21 to 23 °C.

Results

Nominal concentrations (mg/l):	0 (control), 0.18, 0.32, 0.56, 1.0, and 1.8 mg/l
Measured concentrations (mg/l):	No
Unit:	mg/l
Element value:	96-hour LC_{50}
Statistical results:	96-hour LC_{50} = 0.43 mg/l (95% confidence limits: 0.35 and 0.53 mg/l)
Remarks:	The highest concentration causing no mortality (no observed effect concentration) after 96 hours was 0.32 mg/l. 100% mortality occurred in the 0.56, 1.0 and 1.8 mg/l treatment groups. In addition, at concentrations of 0.56 and 1.0 mg/l, fish showed reduced activity from 4 hours after initiation until they died. The following LC_{50} values at earlier exposure times were calculated: 26-hour LC_{50} = 0.55 mg/l (0.47 – 0.64 mg/l) 48-hour LC_{50} = 0.49 mg/l (0.41 – 0.58 mg/l) 72-hour LC_{50} = 0.49 mg/l (0.41 – 0.58 mg/l) The quality of the batch of fish used in the test was checked by means of a test with a reference substance (potassium dichromate). Results were in accordance with expected criteria.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Mark, U. and E. E. Hantink-de Rooij. 1990. Acute Toxicity of [CAS RN 68910-93-0] to Fish. Report number T 90-2-1.9. Akzo Research Laboratories, Arnhem, The Netherlands.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	150
Remarks:	

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Amides, coco, N,N-bis(hydroxyethyl) (CAS RN 68603-42-9)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	German Standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on microcrustaceans (*Daphnia*-Shorttime-Test)(L11); Corresponds to OECD Guideline 202, Part 1.
Test type:	Static
GLP:	Not stated
Year:	1999
Analytical procedures:	Not stated
Species/Strain/Supplier:	*Daphnia magna*
Test details:	Static
Statistical methods:	Not stated
Remarks:	Approximately 20 daphnids per concentration were exposed to a range of concentrations of the test substance in water for 24 hours. Immobilities (loss of ability to swim) were recorded. The following endpoints were determined: EC_0 = highest test concentration having no immobility EC_{50} = concentration showing 50% immobility EC_{100} = lowest test concentration having 100% immobility.

Results

Nominal concentrations (mg/l):	Not stated
Measured concentrations (mg/l):	Not stated
Unit:	mg active matter/l
EC_{50} (24-hour):	3.3 mg active matter/l
Remarks:	In addition to the $EC_{50,}$ the following endpoints were determined: EC_0 = 2.0 mg active matter/l EC_{100} = 5.6 mg active matter/l Results were given in a one-page summary report.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Reliable with restriction; basic data given, comparable to guidelines/standards.

References

Steber, J. and H. Berger. 1999. Biological Research and Product Safety/Ecology: Report number 1986/2497. Henkel KGaA, Duesseldorf, Germany.

Steber, J. and H. Berger. 1999. Biological Research and Product Safety/Ecology: unpublished results; Test substance registration number Fi 6650. Henkel KGaA, Duesseldorf, Germany.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	138
Remarks:	

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Amides, coco, N,N-bis(hydroxyethyl) (CAS RN 68603-42-9)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Test methodology followed: Peltier, W. H. and C. W. Weber, EPA/600/4-85/013, 1985, U. S. EPA Environmental Monitoring and Support Laboratory, Cincinnati, Ohio
Test type:	Static
GLP:	No
Year:	1986
Analytical procedures:	No
Species/Strain:	*Daphnia pulex*
Test details:	Static
Statistical methods:	LC_{50} values determined using the trimmed Spearman-Karber analysis of acute toxicity data (Hamilton, M. A., R. C. Russo and R. V. Thurston. 1977. Environ. Sci. Technol. 11:714-718)
Remarks:	Dilution water hardness ranged from 35 – 40 mg/l as $CaCO_3$. Final dissolved oxygen and pH measurements ranged from 3.7 – 7.5 mg/l and from 7 – 8, respectively, for the highest test concentration. Temperature was maintained at 20 – 21 °C.

Results

Nominal concentrations (mg/l):	Not stated
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
LC_{50} (48-hour):	Two tests were run, the results of each were: 2.15 mg/l 2.64 mg/l
Remarks:	48-hour LC_{50} = 2.15 and 2.64 mg/l.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2C
Remarks:	Reliable with restrictions; comparable to guideline study with acceptable restrictions.

References

Moore, S. B., R. A. Diehyl, J. M. Barnhardt and G. B. Avery. 1986. Acute and Chronic Aquatic Toxicities of Textile Surfactants. Book of Papers: 1986 International Conference & Exhibition, AATCC. October 28 - 31. pp. 290 - 293. Atlanta, GA, U. S.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	141
Remarks:	

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Amidoamine (CAS RN 71820-35-4; Fatty acids, tall-oil, low boiling, reaction products with 1-piperzineethanamine)
Purity:	100%
Remarks:	

Method

Method/Guideline followed:	OECD Guideline 202 and EEC Method C.2
Test type:	Static
GLP:	Yes
Year:	1993
Analytical procedures:	Not stated
Species/Strain:	*Daphnia magna*/I.R.CH.A.
Test details:	Static
Statistical methods:	Thompson, W. R. 1947. The use of moving averages and interpolation to estimate median – effective dose. Bact. Reviews. II, 115 - 145
Remarks:	The experiment measured the acute toxicity of the test substance to *Daphnia magna* in a 48-hour static exposure test. Daphnids were cultured at the laboratory in reconstituted water. They were fed daily with a suspension of mixed algae. Gravid adults were isolated 24 hours prior to initiation; young daphnids produced overnight were used for testing. Groups of daphnids were exposed to nine concentrations of the test substance and a dilution water control. The nominal test concentrations were 0 (control), 0.10, 0.18, 0.32, 0.56, 1.0, 1.8, 3.2, 5.6 and 10 mg/l. Exposure solutions were prepared in reconstituted water. The test material was suspected to adsorb to glassware and so saturation of the adsorption sites was achieved by soaking the test vessels overnight prior to the start of the test with the test solutions. At 0-hours, the test vessels were emptied, rinsed with the solution to be tested and then refilled with the fresh test solution. Treatments were replicated twice with 10 daphnids per replicate (20 daphnids per experimental group). Test vessels were glass jars containing 200 ml of solution and covered to reduce evaporation. A 16-hour light/8-hour dark photoperiod was provided during testing. Dissolved oxygen (DO) and water pH were measured at the start and at test termination. Temperature was recorded daily. The target test temperature was 21 °C. Dissolved oxygen ranged from 7.9 – 8.4 mg/l, pH ranged from 7.8 – 7.9, and

temperature remained at 21 °C during the test. Daphnids were considered immobilized if they were unable to swim for approximately 15 seconds after gentle agitation. Effect concentrations were based on nominal concentrations.

Results

Nominal concentrations (mg/l):	0 (control), 0.10, 0.18, 0.32, 0.56, 1.0, 1.8, 3.2, 5.6, and 10
Measured concentrations (mg/l):	No
Unit:	mg/l
EC_{50} (48-hour):	0.30 mg/l (95% confidence limits, 0.26 – 0.34 mg/l)
NOEC (48-hour):	0.18 mg/l
Statistical results:	Described above
Remarks:	The 24-hour EC_{50} = 0.52 mg/l, with 95% confidence limits of 0.46 and 0.59 mg/l. The 24-hour NOEC = 0.32 mg/l. 100% immobilization occurred in the 0.56, 1.0, 1.8, 3.2, 5.6, and 10 mg/l treatments, 60% immobilization occurred in the 0.32 mg/l treatment. No immobilized daphnids were found at 0 (control), 0.10 and 0.18 mg/l.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Sewell, I. G. and D. Grant-Salmon. 1993. The Acute Toxicity of [CAS RN 71920-35-4] to *Daphnia magna*. SafePharm Laboratories, Derby, UK.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	151
Remarks:	

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	Amides, coco, N-(hydroxyethyl) (CAS RN 68140-00-1)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	German Standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the inhibitory effect of water constituents on green algae (algae growth-inhibition test (L9); DIN 38412 part 9; methods correspond to OECD Guideline 201
Test type:	Static
GLP:	Not stated
Year:	1998
Species/Strain/Supplier:	*Scenedesmus subspicatus*
Element basis:	Determined on cell biomass.
Exposure period:	72 hours
Analytical monitoring:	Not stated
Statistical methods:	Not stated
Remarks:	Algae exposed to a range of concentrations (three replicates/concentration) in a mineral nutrient solution for 72 hours. Cell counts were made daily and treatment levels were compared to the control group.

Results

Nominal concentrations (mg/l):	Not stated
Measured concentrations (mg/l):	Not stated
Unit:	mg active matter/l
Element value:	72-hour E_bC_{50}
Result:	72-hour E_bC_{50} = 1.1 mg active matter/l
Satisfactory control response:	Unknown
Statistical results:	72-hour E_bC_{50} = 1.1 mg active matter/l
Remarks:	Additional endpoints determined in the study included: 72-hour E_bC_0 = 0.3 mg active matter/l 72-hour E_bC_{100} = 8.7 mg active matter/l Results were given in a one-page summary report.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Reliable with restrictions; basic data given, comparable to guidelines/standards.

References

H. Berger and Guhl. 1998. Biological Research and Product Safety/Ecology: Unpublished Results; Test Substance Registration number 6648. Henkel KGaA, Duesseldorf, Germany.

Other

Last changed:	July 21, 2000
Order number for sorting:	118
Remarks:	

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Erucamide (CAS RN 112-84-5)
Purity:	100% commercial product (99% total amide)
Remarks:	Complete characterization provided in report

Method

Method/Guideline followed:	OECD Guideline 202
Test type:	Static-renewal
GLP:	Yes
Year:	1996
Analytical procedures:	Yes, GC/FID
Species/Strain:	*Daphnia magna*/Clone 5
Test details:	Static-renewal
Statistical methods:	Analysis of Variance and Dunnett's Test, as appropriate
Remarks:	The experiment measured the survival and reproduction of *Daphnia magna* over a 21-day exposure to the test and control substances. Daphnids were cultured in the laboratory using Elendt M7 medium and a daily feeding regiment of green algal cells (*Chlorella vulgaris*). Four experimental groups: control (Elendt M7 medium), solvent control (0.1 ml methanol/l), 33 µg/l, and 100 µg/l (nominal concentrations) were used in a static-renewal exposure system. All test solutions were prepared with Elendt M7 medium. Replicate test vessels consisted of 4 oz glass bottles containing 100 ml of test solution. There were 10 replicates per experimental group. On the day of test initiation, neonate daphnids were removed from cultures and placed in a crystallizing dish containing Elendt M7 medium. One daphnid was placed in each replicate test vessel, and each vessel was randomly placed in the testing area. Light intensity was not measured, but ambient laboratory lighting was provided with a photoperiod of 16 hours light/8 hours dark. Each day, test solutions were renewed, and the daphnids were fed 1.7×10^5 cells/ml of *Chlorella vulgaris*. Adult survival and reproduction was assessed each day and neonates were removed daily. The pH, dissolved oxygen (DO) and total hardness (as mg/l $CaCO_3$) were measured on test days 0, 1, every Tuesday and Friday and on day 21. Means and ranges for temperature, water pH, DO and total hardness were 19.7 °C (14.5 – 25.0 °C), 7.6 (7.2 – 8.1), 8.2 mg/l (4.5 – 9.3 mg/l) and 245 mg/l (234 – 256 mg/l) as $CaCO_3$, respectively. Concentrations of the test substance in exposure solutions

were measured on test days 0, 1, 5, 9, 12, 16 and 19 in both the old and the new solutions. Effect concentrations were based on mean measured concentrations.

Results

Nominal concentrations:	0 (control), 0 (solvent control), 33 and 100 µg/l
Measured concentrations:	< 0.1, < 0.1, 23.2 and 79.7 µg/l
Unit:	µg/l
NOEC:	NOEC = 80 µg/l. No inhibitory effects of the test substance were measured at the highest test concentration. Thus, the NOEC was empirically estimated to be 80.0 µg/l.
Remarks:	Analyses of the test solutions indicated that concentrations of the test substance in the fresh solutions averaged 83.5% of nominal and old solutions averaged 65.2% of nominal. A malfunction in a temperature controller caused a deviation from the specified temperature range during the test. This was not considered to have had a significant impact on the outcome of the study.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Marshall, S. J. and S. R. Harding. 1996. The Chronic Toxicity of UNISLIP 1753 to *Daphnia magna*. Study number CT/N25/02. Unilever Research, Port Sunlight Laboratory, Merseyside, UK.

Other Available Reports

Other

Last changed:	July 20, 2000
Order number for sorting:	35
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Armid 18 (CAS RN 124-26-5; Stearamide)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	FHSA, 16 CFR 1500.3(c)(2)(i)
Type:	LD_{50} limit test
GLP:	Yes
Year:	1983
Species/Strain:	Sprague-Dawley rat
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	Corn oil
Route of administration:	Oral gavage
Remarks:	Five male rats (217 to 234 g) and five female rats (203 to 230 g) were administered the test material as a 50% w/v formulation in corn oil at a dosage of 10.0 g/kg body weight. All animals were fasted from feed for approximately 17 hours prior to treatment. Animals were observed for gross signs of toxicity and death at approximately 1 ½ to 2, 2 ½ to 3 and 5 ¾ to 6 ¼ hours following treatment and once daily thereafter for 14 days. At the end of the 14-day observation period the rats were weighed, killed and a gross necropsy was performed.

Results

Value:	LD_{50} > 10 g/kg
Number of deaths:	0
Remarks:	No deaths occurred. No clinical changes were observed in the female rats. Transient diarrhea was observed in the male rats on the day of dosing. All rats gained weight. Gross necropsies at the end of the study revealed no gross alterations.

Conclusions

Remarks:	The material is not classified as toxic by oral administration (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1C
Remarks:	Reliable without restriction; test procedure according to national standards.

References

Conine, D. L. Acute Oral Toxicity Screen in Rats of Armid 18. 1983. Report number 83-0488-21. Hill Top Research, Inc., Cincinnati, OH, U. S.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	54
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Oleamide DEA (CAS RN 301-02-0; Oleamide)
Purity:	Concentration = 100%
Remarks:	

Method

Method/guideline followed:	Not stated
Type:	LD_{50}
GLP:	Not stated
Year:	Not stated
Species/Strain:	Sprague Dawley Rats
Sex:	Male and Female
No. of animals per sex per dose:	5
Vehicle:	None – dosed undiluted
Route of administration:	Oral gavage
Remarks:	Five male and five female rats per dose group were administered a singe oral dose of the test substance. Multiple dose levels were used to determine an LD_{50}. Animals were fasted from feed 16 hours prior to dose administration and allowed only water. Rats were observed for general health and activity one hour after administration and daily for 14 days.

Results

Value:	LD_{50} = 12.4 ml/kg 95% confidence limits = 11.1 – 13.9 ml/kg
Number of deaths:	Not stated
Remarks:	LD calculated using the method of Weil.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2B
Remarks:	Reliable with restrictions: basic data given, comparable to guidelines.

References

Acute Oral Toxicity (LD_{50}) of Oleamide DEA to Rats. CTFA Code number 2-32-118. CIR Safety Data Test Summary Response Form.

Other Available Reports

Other

Last changed: July 24, 2000
Order number for sorting: 77b
Remarks:

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Erucamide (CAS RN 112-84-5)
Purity:	Approximately 99%
Remarks:	

Method

Method/guideline followed:	EEC Test method B.1 as described in the Annex of EEC Directive 84/449
Type:	LD_{50} limit test
GLP:	Yes
Year:	1988
Species/Strain:	Wistar rat
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	Corn oil
Route of administration:	Oral gavage
Remarks:	Five male and five female young adult rats (9 weeks old at study start) were utilized for this study. Animals were fasted overnight prior to dosing until approximately three hours after administration of the test substance. The test substance was suspended in corn oil and administered twice within 24 hours. The dose level was 5000 mg/kg body weight (dosed twice at 2500 mg/kg) and each time the dose volume was 10 ml/kg body weight. Clinical observations were performed on the day of dosing approximately once every two hours and once daily thereafter for 14 days. Individual body weights were measured weekly. At the end of the study all animals were killed by CO_2 inhalation and subjected to a necropsy.

Results

Value:	LD_{50} > 5000 mg/kg
Number of deaths:	0
Remarks:	No deaths occurred and no signs of systemic toxicity were observed during the 14-day observation period. All animals showed body weight gain. Macroscopic examination of animals at termination did not reveal any abnormalities that were considered to be treatment-related.

Conclusions

Remarks:	Under the conditions of this study it is concluded that the test substance has no toxic effect when administered as two oral doses within 24 hours to the rat at a total dose level of

5000 mg/kg body weight (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1A
Remarks: Reliable without restriction; guideline study.

References

Reijnders, J. B. J. Acute Oral Toxicity of UNISLIP 1753 in Rats. 1988. Report number 0812/1044. RCC NOTOX B.V., 's-Hertogenbosch, The Netherlands.

Other Available Reports

Other

Last changed: July 24, 2000
Order number for sorting: 36a
Remarks:

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Armid HT (CAS RN 61790-31-6; Amides, tallow, hydrogenated)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	OECD Guideline No. 401 "Acute Oral Toxicity"
Type:	LD_{50} limit test
GLP:	No
Year:	1985
Species/Strain:	Sprague-Dawley rat
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	Methylcellulose
Route of administration:	Oral gavage
Remarks:	A preliminary study was conducted using groups of two male and two female rats at dose levels of 0.5, 1.0 and 5.0 g/kg. Based on the results of this preliminary study, a group of five male and five female rats (approximately 4 – 6 weeks in age, 100 – 117 g body weight) were administered a single dose of the test substance at a dose level of 5.0 g/kg body weight. The test substance was prepared as a 50% w/v suspension in 1% methylcellulose and administered at a volume not exceeding 10.0 ml/kg. Animals were acclimated to the experimental environment for at least five days prior to study initiation. They were fasted from food overnight prior to dosing and for four hours post-dose. Animals were observed soon after dosing, then at frequent intervals for the remainder of the day of dosing. Animals were observed at least twice daily thereafter for 14 days for mortality and toxicity. Animals were subjected to a complete gross necropsy following the 14-day observation period.

Results

Value:	LD_{50} > 5 g/kg body weight
Number of deaths:	0
Remarks:	All animals survived. Clinical signs including piloerection and hunched posture were observed in all animals until day 5. After this time all animals appeared normal and gained weight through day 14. Necropsy yielded no abnormal findings.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions; acceptable, well-documented study report which meets basic scientific principles.

References

Kynoch, S. R. 1985. Acute Oral Toxicity to Rats of Armid HT. Report number 85268D/AKZ 190/AC. Huntingdon Research Centre, Cambridgeshire, UK.

Other Available Reports

Other

Last changed:	July 25, 2000
Order number for sorting:	160a
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Carsamide SAL-7 (CAS RN 120-40-1; Dodecanamide, N,N-bis(2-hydroxyethyl)-)
Purity:	70%
Remarks:	Composition included 25% water and 5% DEA

Method

Method/guideline followed:	According to the procedure suggested in: Hagan, E. C. 1959. Acute Toxicity; Appraisal of the safety of chemicals in foods, drugs and cosmetics. 17 – 25.)
Type:	LD_{50} limit test
GLP:	No
Year:	1979
Species/Strain:	Wistar albino rat
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Oral gavage
Remarks:	Five male and five female rats (182 – 220 g) were administered a single dose of the test substance in aqueous solution at a level of 5.0 g/kg body weight. The test substance was used as received. Animals were acclimated to standard laboratory conditions for a minimum of seven days and fasted overnight prior to dosing. Animals were observed for signs of pharmacologic activity and drug toxicity 1, 3, 6 and 24 hours post-dose and once daily thereafter for 14 days. Animals were subjected to a complete gross necropsy following the 14-day observation period.

Results

Value:	LD_{50} > 3.5 g /kg active ingredient.
Number of deaths:	3 (2 female, 1 male)
Remarks:	One male and two females died by day 4. Slight depression was observed in eight of the ten animals tested through day 3, after which time the animals that survived the 14-day observation period appeared normal and gained body weight. Necropsy observations included pyloric and intestinal mucosa severely reddened in one female that died. No other gross changes were observed in any other animals. The LD_{50} of the original solution (70%) was 0.5 g/kg.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2C
Remarks:	Reliable with restrictions; comparable to guideline study with acceptable restrictions.

References

Lewis, C. A. and A. L. Palanker. Acute Oral Toxicity (Rat). 1979. Report number 7936-10. Consumer Product Testing, Fairfield, NJ, U. S.

Other Available Reports

Other

Last changed:	August 14, 2000
Order number for sorting:	45b
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Monamid 716 (CAS RN 120-40-1; Dodecanamide, N,N-bis(2-hydroxyethyl)-)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Testing guideline not reported (According to procedure suggested in: Hagan, E. C. 1959. Acute Toxicity; Appraisal of the safety of chemicals in foods, drugs and cosmetics. 17 – 25.))
Type:	LD_{50} limit test
GLP:	Not stated
Year:	1976
Species/Strain:	Rats/Wistar
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	Not stated
Route of administration:	Oral gavage
Remarks:	Five male and five female rats (188 - 284 g) were administered a single oral dose of the test substance at a level of 5.0 ml/kg body weight after being fasted overnight. Animals were observed for signs of pharmacologic activity and drug toxicity at 1, 3, 6 and 23 hours post-dose. Observations were made daily thereafter for a total of 14 days. A complete gross necropsy was performed at the end of the 14-day observation period.

Results

Value:	LD_{50} > 5 ml/kg
Number of deaths:	0
Remarks:	No deaths occurred and no clinical changes were observed in the male or female rats throughout the 14-day observation period. All rats gained weight.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions; acceptable, well-documented publication/study report which meets basic scientific principles.

References

Palanker, A. L. Acute oral toxicity. 1976. Report number 7667- 8/8. Consumer Product Testing Company, Inc., Fairfield, NJ, U. S.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	46A
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Monamid 705 (CAS RN 68603-42-9; Amides, coco, N, N-bis(hydroxyethyl))
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Not stated
Type:	LD_{50} limit test
GLP:	Not stated
Year:	1977
Species/Strain:	Rats/Wistar
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Oral gavage
Remarks:	Five male and five female rats (206 - 242 g) were administered a single oral dose of the test substance at a level of 5.0 g/kg body weight. The material was used as received. Animals were observed for 14 days.

Results

Value:	$LD_{50} > 5$ g/kg
Number of deaths:	0
Remarks:	No deaths occurred and no clinical changes were observed in the male or female rats throughout the 14-day observation period.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Reliable with restrictions; basic data given, comparable to guidelines/standards.

References

Lewis, C. A. and A. L. Palanker. 1977. Acute Oral Toxicity (rat). Report number 77325. Consumer Product Testing Company, Inc., Fairfield, NJ, U. S.

Other Available Reports

Other

Last changed:	July 25, 2000
Order number for sorting:	144b
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Carsamide SAC (CAS RN 68603-42-9; Amides, coco, N, N-bis(hydroxyethyl))
Purity:	95% *(this was handwritten on the article)*
Remarks:	Test substance also consisted of 5% DEA *(this was handwritten on the article).*

Method

Method/guideline followed:	Procedure suggested in: Hagan, E. C. 1959. Acute Toxicity; Appraisal of the safety of chemicals in foods, drugs and cosmetics. 17 – 25.
Type:	LD_{50} limit test
GLP:	No
Year:	1977
Species/Strain:	Albino rat
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Oral gavage
Remarks:	Five male and five female rats (150 – 300 g) were administered a single dose of the test substance at a level of 5.0 g/kg body weight. The test substance was used as received. Animals were acclimated to standard laboratory conditions for a minimum of seven days and fasted overnight prior to dosing. Animals were observed for signs of pharmacologic activity and drug toxicity 1, 3, 6 and 24 hours post-dose and once daily thereafter for 14 days. Animals were subjected to a complete gross necropsy following the 14-day observation period.

Results

Value:	$LD_{50} > 5.0$ g/kg
Number of deaths:	1
Remarks:	One male died by day 6. Slight depression was observed in all animals tested at 24 hours post-dose, after which time all animals appeared normal. All animals that survived the 14-day observation period gained body weight. No necropsy observations were reported.

Conclusions

Remarks: The test substance may not be considered an orally toxic material to rats under the conditions of this test (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2A
Remarks: Reliable with restrictions; acceptable, well-documented study report which meets basic scientific principles.

References

Palanker, A. L. Acute Oral Toxicity (Rat). 1977. Report number 7774-2. Consumer Product Testing Company, Inc., Fairfield, NJ, U. S.

Other Available Reports

Other

Last changed: July 25, 2000
Order number for sorting: 144c
Remarks:

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Monamid 150-ADD (CAS RN 68603-42-9; Amides, coco, N, N-bis(hydroxyethyl))
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Testing guideline not reported (According to procedure suggested in: Hagan, E. C. 1959. Acute Toxicity; Appraisal of the safety of chemicals in foods, drugs and cosmetics. 17 – 25.)
Type:	LD_{50} limit test
GLP:	Not stated
Year:	1976
Species/Strain:	Wistar rat
Sex:	Male and Female
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Oral gavage
Remarks:	Five male and five female rats (176 - 196 g) were administered a single dose of the test substance at a level of 5.0 ml/kg body weight. The material was used as received, diluted in solvent where appropriate. Animals were fasted overnight prior to dosing. Animals were observed for signs of pharmacologic activity and drug toxicity at 1, 3, 6 and 24 hours post-dose. Daily observations were made for 14 days thereafter. Animals were sacrificed and a complete gross necropsy was performed following the 14-day observations period.

Results

Value:	LD_{50} >5 ml/kg
Number of deaths:	All animals survived.
Remarks:	All animals appeared normal throughout the 14 day except for slight depression seen in all animals at the 24-hour post-dose observation period.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions; acceptable, well-documented publication that meets basic scientific principles.

References

Palanker, A. L. Acute Oral Toxicity (Rat). 1976. Report number 7667-4/8. Consumer Product Testing Company, Inc., Fairfield, NJ, U. S.

Other Available Reports

Other

Last changed:	July 25, 2000
Order number for sorting:	145
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Amides, coco, N-(hydroxyethyl) (CAS RN 68140-00-1)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Not stated
Type:	LD_{50} limit test
GLP:	Not stated
Year:	1972
Species/Strain:	Wistar rat
Sex:	Male
No. of animals per sex per dose:	10
Vehicle:	None
Route of administration:	Oral gavage
Remarks:	Ten young adult male rats were administered a single dose of the test substance at a level of 5000 mg/kg body weight. Animals were fasted prior to dosing. Animals were observed for 8 days.

Results

Value:	LD_{50} > 5.0 g/kg
Number of deaths:	0
Remarks:	All animals survived the 8-day observation period and no adverse effects were observed. With respect to the determined LD_{50} value, it is assumed that the LD_{50} value for female rats also exceeds the limit dose of > 2000 mg/kg body weight (author of the report).

Conclusions

Remarks:	This test substance is not toxic as defined in the guidelines (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; summary of German report.

References

Sterzel, W. and T. Broschard. 1972. Evaluation of Acute Oral Toxicity. Report number TBD 720033. Henkel KGaA, Duesseldorf, Germany.

Other Available Reports

Other

Last changed:	July 25, 2000
Order number for sorting:	119
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Unamide CDX (CAS RN 68140-00-1; Amides, coco, N-(hydroxyethyl))
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Not stated
Type:	LD_{50}
GLP:	No
Year:	1976
Species/Strain:	Rat/Strain not stated
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Oral gavage
Remarks:	Six groups of male and female young adult albino rats (200 – 300 g) were administered a single dose of the test substance at levels of 1.0, 2.0, 4.0, 8.0, 16.0 or 32.0 g/kg. The test substance was used as received. Animals were fasted for 24 hours prior to dosing and both sexes were equally distributed. Animals were observed daily for two weeks post-dose. No postmortem, or histopathology examinations were performed in this study.

Results

Value:	LD_{50} = 7.4 g/kg (95% Confidence Limits = 5.4 – 10.4 g/kg)
Number of deaths:	3/5 at 8.0 g/kg dose level 5/5 at 16.0 and 32.0 g/kg dose levels
Remarks:	Animals in the 1.0 g/kg dose group showed no signs of toxicity from the test substance. Lacrimation was observed 24 to 36 hours post-dose in animals treated with 2.0 g/kg of the test substance. Observations of animals treated with 4.0 g/kg of the test substance included nasal hemorrhage and unkempt coats. Nasal hemorrhage, lacrimation, diarrhea, sluggish, impaired locomotion and weight loss were observed in animals treated with 8.0 and 16.0 g/kg of the test substance. Lethargy, lacrimation, nasal hemorrhage, moderate to severe diarrhea and dirty unkempt coats were observed in animals treated with 32.0 g/kg of the test substance. The test substance was equally toxic to males and females.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2C

Remarks: Reliable with restrictions; comparable to guideline study with acceptable restrictions.

References

Wallace, J. M. 1976. Toxicity Studies for Lonza Inc. Bio-Toxicology Laboratories, Inc., Moorestown, NJ, U. S.

Other Available Reports

Other

Last changed: July 25, 2000

Order number for sorting: 120a

Remarks:

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	10% Monamid ACC (CAS RN 68140-00-1; Amides, coco, N-(hydroxyethyl))
Purity:	Not stated
Remarks:	Aqueous solution

Method

Method/guideline followed:	Not stated
Type:	LD_{50}
GLP:	No
Year:	1971
Species/Strain:	CFE rat
Sex:	Male and female
No. of animals per sex per dose:	1 and 5
Vehicle:	None
Route of administration:	Oral gavage
Remarks:	Two rats (approximately 140 g) were administered a single dose of the test substance at dose levels of 5.0, 20, 30, or 40 ml/kg body weight, and ten rats (approximately 140 g) administered a single dose of the test substance at a dose of 50 ml/kg body weight. The test substance was used as received. Animals were fasted from food for 18 hours prior to dosing. Animals were observed for 5 days post-dose for signs of toxicity.

Results

Value:	LD_{50} > 5 g/kg active ingredient
Number of deaths:	0
Remarks:	All animals survived and did not exhibit any visible toxic effects. The LD_{50} of the original solution (10%) was > 50 ml/kg.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Reliable with restrictions; basic data given, comparable to guidelines/standards.

References

Wolven, A. M. and I. Levenstein. 1971. Determination of Oral LD_{50} in Rats. Report number 14861. Leberco Laboratories, Roselle Park, NJ, U. S.

Other Available Reports

Other

Last changed:	July 25, 2000
Order number for sorting:	120b
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Monamid ACC Lot #1876 (CAS RN 68140-00-1; Amides, coco, N-(hydroxyethyl))
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Acute toxicity procedure suggested in: Hagan, E. C. 1959. Acute Toxicity; Appraisal of the safety of chemicals in foods, drugs and cosmetics. 17 – 25.)
Type:	LD_{50} limit test
GLP:	No
Year:	1976
Species/Strain:	Wistar rat
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Oral gavage
Remarks:	Five male and five female rats (172 - 290 g) were administered a single oral dose of the test substance at a level of 5.0 ml/kg body weight. The test substance was used as received. Animals were fasted from food overnight prior to dosing. Animals were observed 1, 3, 6 and 24 hours post-dose and once daily thereafter for 14 days for mortality, toxicity and pharmacological effects. Animals were subjected to a complete gross necropsy following the 14-day observation period.

Results

Value:	LD_{50} > 5 ml/kg
Number of deaths:	0
Remarks:	All animals survived. All animals appeared normal and gained weight through day 14.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions; acceptable, well-documented study report which meets basic scientific principles.

References

Palanker, A. L. Acute Oral Toxicity (Rat). 1976. Report number 7667-1/8. Consumer Product Testing Company, Inc., Fairfield, NJ, U. S.

Other Available Reports

Other

Last changed:	July 25, 2000
Order number for sorting:	121a
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Amides, C12-18, N,N-bis(hydroxyethyl) (CAS RN 68155-06-6)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Not stated
Type:	LD_{50} limit test
GLP:	Not stated
Year:	1971
Species/Strain:	Wistar rat
Sex:	Male
No. of animals per sex per dose:	10
Vehicle:	Distilled water
Route of administration:	Oral gavage
Remarks:	Ten male rats were administered a single dose of the test substance in distilled water at a level of 10.0 g/kg body weight. Animals were fasted prior to dosing. Animals were observed for 8 days.

Results

Value:	LD_{50} > 10.0 g/kg
Number of deaths:	1
Remarks:	One animal died 24 hours post-dose without specific symptoms of intoxication. All other animals survived the study. With respect to the determined LD_{50} value, it is assumed that the LD_{50} value for female rats also exceeds the limit dose of 2000 mg/kg body weight (author of report).

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; summary of German report.

References

Sterzel, W. and T. Broschard. 1999. Evaluation of Acute Oral Toxicity. Report number 710070. Henkel KGaA, Duesseldorf, Germany.

Other Available Reports

Other

Last changed: July 27, 2000
Order number for sorting: 143
Remarks:

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	*Sanitized report – chemical name not specified.* (CAS RN 71820-35-4; Fatty acids, tall-oil, low boiling, reaction products with 1-piperzineethanamine)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Not stated
Type:	LD_{50}
GLP:	Yes
Year:	1983
Species/Strain:	Sprague-Dawley rat
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	Distilled water
Route of administration:	Oral gavage
Remarks:	A preliminary study was run with 1 male and 1 female per group was administered the test substance at 250, 500, 1000, 3000 or 5000 mg/kg. Based on the results of this dose range-finding test, dose levels of 3000, 4000 and 5000 mg/kg of the test substance were selected to determine the LD_{50} of the test substance. Five male and 5 female rats (145 – 231 g) per group were utilized for this study. Animals were fasted for 16 hours prior to dosing. The test substance was prepared in distilled water before administration and each group was does at a constant dose volume of 20 ml/kg. Animals were observed for 14 days post-dose. Individual body weights were measured weekly, or at death. At the end of the study all surviving animals were sacrificed and subjected to a necropsy.

Results

Value:	LD_{50} for males = 3610 mg/kg (95% Confidence Limits = 2919 – 4464 mg/kg) LD_{50} for females = 4260 mg/kg (95% Confidence Limits = 3975 – 4565 mg/kg)
Number of deaths:	3 males at 3000 mg/kg dose level 3 males and 3 females at 4000 mg/kg dose level 3 males and 4 females at 5000 mg/kg dose level
Remarks:	All deaths occurred within 5 days post-dose. Clinical signs noted in each dose group included hunched appearance, hypokinesia, ataxia, prostration, sedation, piloerection,

soiled coat, red-stained urine, diarrhea, epistaxis, excess salivation, dyspnea, chromodacryorrhea and/or alopecia through day 14. All surviving animals gained weight by day 14. Macroscopic examination of animals at termination revealed pale/red lungs, spongy/congested lungs, gas-filled stomach/gut, autolysis, yellow or red contents/fluid in guts and/or white fluid in thorax. Due to the unusual mortality pattern for males, it was not possible to determine an LD_{50} value using probit analysis. Therefore, after consideration of the dose range-finding results and the female mortality pattern, the assumption was made that had a further group been dosed at a dose level of 1000 mg/kg no deaths would have occurred. An LD_{50} value was calculated base on this assumption.

Conclusions

Remarks: Under the conditions of this study it is concluded that the test substance may be considered to be slightly toxic to rats (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1B
Remarks: Reliable without restriction; comparable to guideline study.

References

Cuthbert, J. A and K. J. D'Arcy-Burt. 1983. Toxicity Tests on Product [CAS RN 71820-35-4]. Inveresk Research International, Musselburgh, UK.

Other Available Reports

Other

Last changed: July 25, 2000
Order number for sorting: 152
Remarks:

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Armid HT (CAS RN 71820-35-4; Fatty acids, tall-oil, low boiling, reaction products with 1-piperzineethanamine)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	
Type:	LD_{50}
GLP:	Yes
Year:	1985
Species/Strain:	Rats/Sprague-Dawley
Sex:	Male and female
No. of animals per sex per dose:	2
Vehicle:	Not stated
Route of administration:	Oral gavage
Remarks:	Two male and two female rats (100 - 146 g, approximately four to six weeks of age) per group were administered a single oral dose of the test substance at a level of 25, 200, 2000 or 5000 mg/kg body weight. The test substance was administered as supplied at a volume of 0.21, 2.1 and 5.2 ml/kg for the 200, 2000 and 5000 mg/kg groups, respectively. The 25 mg/kg group were administered the test substance as a 25% w/v solution in distilled water (prepared on the day of dosing) and administered at a volume of 0.1 ml/kg. Animals were fasted overnight prior to dosing and approximately four hours after dosing. Animals were observed soon after dosing, at frequent intervals throughout the day of dosing and for 14 days subsequent to dosing. Body weights were obtained on Days 1 (day of dosing), 4, 8 and 15. A complete gross necropsy was performed on Day 15.

Results

Value:	LD_{50} > 5000 mg/kg
Number of deaths:	0
Remarks:	No deaths occurred at any dose level. Signs of reaction to treatment observed shortly after dosing in all rats were pilo-erection and abnormal body carriage. These signs were accompanied by abnormal gait in all rats a 200 mg/kg and above, diarrhea in all rats at 2000 and 5000 mg/kg, lethargy in all rats at 5000 mg/kg and abdominal distention in one female rat at 200 mg/kg. All animals recovered by days 4

or 8. Body weight loss on Day 4 and a low body weight gain on Day 8 were recorded for one female rat at 200 mg/kg however, a normal weight gain was observed on day 15. All other animals gained weight throughout the 15 days of study. No gross lesions were observed at necropsy.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1B
Remarks: Reliable without restriction; comparable to guideline study.

References

Kynoch, S. R. Acute Oral Toxicity to Rats of Armid HT. 1985. Report number 85268 AKZ190 AC. Huntingdon Research Centre, Cambridgeshire, UK.

Other Available Reports

Other

Last changed: July 25, 2000
Order number for sorting: 153
Remarks:

5.1.2 ACUTE INHALATION TOXICITY

Test Substance

Identity:	Alkanolamide #1 (CAS RN 68155-20-4; Amides, tall-oil fatty, N,N-bis(hydroxyethyl))
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Not stated
Type:	Sensory and pulmonary irritation
GLP:	Not stated
Year:	1994
Species/Strain:	Swiss-Webster mice
Sex:	Male
No. of animals per sex per dose:	4
Vehicle:	None
Route of administration:	Inhalation
Remarks:	Four male mice (24 to 28 g) were used for each experiment. No control animals were used. Each animal was acclimated for 20 minutes to the exposure chamber followed by a 3-hour exposure period. The range of concentrations used was 86-219 mg/m^3. Animals were visually checked for several days following exposure.

Results

Value:	Not stated
Number of deaths:	0
Remarks:	The test article produced sensory irritation later in the exposure at low concentrations. Pulmonary irritation also occurred later in these exposures. These also produced variable affects between animals.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions; acceptable, well-documented publication/study report which meets basic scientific principles.

References

Krystofiak, S. P. 1994. Evaluation of the Respiratory Effects from Components of a Metalworking Fluid in Mice. EPA Document number 88-950000037. University of Pittsburgh, Pittsburgh, PA, U. S.

Other available reports

Other

Last changed:	July 3, 2001
Order number for sorting:	125
Remarks:	

5.1.2 ACUTE INHALATION TOXICITY

Test Substance

Identity:	Acrawax® C (CAS RN 110-30-5; Octadecanamide, N,N'-ethylenebis)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Not stated
Type:	Lung toxicity study
GLP:	Not stated
Year:	1990
Species/Strain:	CD® rat
Sex:	Male
No. of animals per sex per dose:	Not stated
Vehicle:	None
Route of administration:	Inhalation
Remarks:	This study was conducted to examine lung toxicity after an acute 6-hour, nose-only exposure to the test substance. An LC_{50} value was not determined. Groups of male rats (8 weeks old) were exposed to dust aerosols of the test substance at 112 mg/m^3 for 6 hours. During exposure, samples of atmospheric test substance were taken from the animal breathing zone to determine the mass median aerodynamic diameter (MMAD) and % of particles less than 10 µm aerodynamic diameter. Fluids and cells from dust-exposed animals and age-matched sham controls were recovered using bronchoalveolar lavage (BAL) and evaluated for cellular and biochemical parameters at 0, 24 and 48 hours, and 8 days and one month post-exposure. Pulmonary macrophages were cultured and studied for *in vitro* and *in vivo* phagocytosis, as well as surface morphology. The lungs of animals exposed to the test substance were fixed for assessment by histopathology, and transmission electron microscopy.

Results

Value:	Not determined
Number of deaths:	0
Remarks:	The MMAD was determined to be 5.2 µm with 72% of particles less than 10 µm. The overall mean atmospheric concentration for Acrawax®C was 112 mg/m^3 $\pm$ 28. A mild and transient inflammatory response at 24 hours post-exposure was observed. BAL levels of lactate

dehydrogenase, alkaline phosphatase and protein were slightly different from controls only at 8 days post-exposure, and had returned to control values by one month of recovery. Test substance exposure had no adverse effects on either morphology or the phagocytic capacity of pulmonary macrophages recovered from exposed animals. There were no histopathologic findings of lung tissue from rats exposed to the test substance.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2A
Remarks: Reliable with restrictions; acceptable, well-documented publication which meets basic scientific principles.

References

Warheit, D. B., M. C. Caarakostats and M. A. Hartsky. 1990. Assessments of Lung Toxicity to Acrawax® C Following Acute Inhalation Exposure. Drug Chem. Toxicol. 13(1):1-18.

Other available reports

Other

Last changed: July 3, 2001
Order number for sorting: 19
Remarks:

5.1.3 ACUTE DERMAL TOXICITY

Test Substance

Identity:	Monamid 716 (CAS RN 120-40-1; Dodecanamide, N,N-bis(2-hydroxyethyl)-)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	A modification of the techniques described in Appraisal of the Safety of Chemicals in Foods, Drugs and Cosmetics, compiled by the staff of the Division of Pharmacology, Food and Drug Administration.
Type:	LD_{50} limit test
GLP:	None stated
Year:	1976
Species/Strain:	Albino Rabbit
Sex:	Male and female
No. of animals per sex per dose:	3
Vehicle:	None
Route of administration:	Dermal
Remarks:	The weight range for the six rabbits used in this study was 2.1 to 2.5 kg. The skin of three rabbits (2 male and 1 females) was abraded. A single dermal application of 2 g/kg was used. The trunk of each animal was then encased in a sleeve of plasticized material to ensure contact of the test material for a 24-hour period. Following the 24-hour exposure period, the sleeve was removed and the animals were observed for mortality, skin response and general behavior for 14 days.

Results

Value:	LD_{50} > 2 g/kg
Number of deaths:	Abraded skin: 0/3 Intact skin: 0/3
Remarks:	No deaths were seen in this study. All animals appeared normal throughout the 14-day post-exposure observation period.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions: acceptable, well-documented publication that meets basic scientific principles.

References

Palanker, A. L. Dermal toxicity. 1976. Report number 7667- 8/8. Consumer Product Testing Company, Inc., Fairfield, NJ, U. S.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	46A
Remarks:	

5.1.3 ACUTE DERMAL TOXICITY

Test Substance

Identity:	Monamid 150-ADD (CAS RN 68603-42-9; Amides, coco, N, N-bis(hydroxyethyl))
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	A modification of the techniques described in Appraisal of the Safety of Chemicals in Foods, Drugs and Cosmetics, compiled by the staff of the Division of Pharmacology, Food and Drug Administration.
Type:	LD_{50} limit test
GLP:	None stated
Year:	1976
Species/Strain:	Albino Rabbit
Sex:	Male and female
No. of animals per sex per dose:	3
Vehicle:	None
Route of administration:	Dermal
Remarks:	The weight range for the six rabbits used in this study was 1.9 to 2.7 kg. The skin of three rabbits (2 male and 1 females) was abraded. A single dermal application of 2 g/kg was used. The trunk of each animal was then encased in a sleeve of plasticized material to ensure contact of the test material for a 24-hour period. Animals were observed immediately after dosing, and at 1, 6 and 24 hours post-dosing. Following the 24-hour exposure period, the sleeve was removed and the animals were observed for mortality, skin response and general behavior for 14 days.

Results

Value:	LD_{50} > 2 g/kg
Number of deaths:	Abraded skin: 0/3 Intact skin: 0/3
Remarks:	No deaths were seen in this study. All animals appeared normal throughout the 24-hour exposure period and the 14-day post-exposure observation period.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions: acceptable, well-documented publication that meets basic scientific principles.

References

Palanker, A. L. Acute Dermal Toxicity (Rabbit). 1976. Report number 7667-4/8. Consumer Product Testing Company, Inc., Fairfield, NJ, U. S.

Other Available Reports

Other

Last changed:	July 25, 2000
Order number for sorting:	145
Remarks:	

5.1.3 ACUTE DERMAL TOXICITY

Test Substance

Identity:	Monamid ACC Lot #1876 (CAS RN 68140-00-1; Amides, coco, N-(hydroxyethyl))
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	A modification of the techniques described in Appraisal of the Safety of Chemicals in Foods, Drugs and Cosmetics, Division of Pharmacology, Food and Drug Administration
Type:	LD_{50} limit test
GLP:	No
Year:	1976
Species/Strain:	Albino rabbit
Sex:	Male and female
No. of animals per sex per dose:	3
Vehicle:	None
Route of administration:	Dermal
Remarks:	Three male and three female rabbits (1.9 - 2.7 kg) were administered a single dose of the test substance at a level of 2.0 g/kg body weight. The test substance was used as received. Prior to dosing the trunk of each animal was clipped free of hair. Three of the animals (two male, one female) were further prepared by introducing epidermal abrasions over the clipped skin surface to enhance penetrability of the test substance through the stratum corneum. After test substance application the trunk of each animal was encased in a sleeve of plasticized material for 24 hours. Following the 24-hour exposure period the sleeve was removed and the skin sites gently cleansed. All animals were observed daily thereafter for 14 days for mortality, skin response and general behavior.

Results

Value:	LD_{50} > 2 g/kg
Number of deaths:	0
Remarks:	All animals survived. All animals appeared normal through day 14. Two females that had abraded skin lost weight (0.01 and 0.25 kg) over the 14-day post-exposure period. All remaining rabbits gained weight through day 14.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions; acceptable, well-documented study report which meets basic scientific principles.

References

Palanker, A. L. Dermal Toxicity (Rabbit). 1976. Report number 7667-1/8. Consumer Product Testing Company, Inc., Fairfield, NJ, U. S.

Other Available Reports

Other

Last changed:	July 25, 2000
Order number for sorting:	121a
Remarks:	

5.4 REPEATED DOSE TOXICITY

Test Substance

Identity:	Erucamide (CAS RN 112-84-5)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Not stated
Test type:	Oral
GLP:	Not stated
Year:	1960
Species:	Rat
Strain:	Wistar
Route of administration:	Oral gavage (stomach tube)
Duration of test:	Other
Doses/concentration levels:	7500 mg/kg of body weight
Sex:	Not stated
Exposure period:	5 days
Frequency of treatment:	Ten doses per day of 1 ml each
Control group and treatment:	Yes (concurrent, treated with distilled water)
Postexposure observation period:	23 Days
Statistical methods:	Not stated
Remarks:	Ten rats weighed approximately 330 grams were used on study. A gel was prepared of the test substance in peanut oil at a concentration to contain 25 grams per 100 ml. Thus each ml contained 250 mg of the test substance. Ten daily doses, approximately 1 ml each, were administered by stomach tube; therefore, the daily intake was approximately 7500 mg/kg body weight. Animals were retained for 23 days following cessation of dosing to observe appetite and appearance. Gross necropsy was performed on the 24th day.

Results

NOAEL (NOEL)	NOEL = 7500 mg/kg
LOAEL (LOEL)	LOEL = 7500 mg/kg
Actual dose received:	approximately 7500 mg/kg
Toxic response/effects:	Described below
Statistical results:	Not stated
Remarks:	None of the rats died. All rats exhibited normal appetite and appearance throughout the study period. No weight loss was observed and no gross pathology or tissue damage was noted. No histopathology was performed and therefore

this study is not adequate to fulfill SIDS requirements for reproductive screening.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2B

Remarks: Reliable with restrictions; basic data given, comparable to guidelines/standards.

References

Molnar, N. M. 1960. Feeding Experiments: Approximate Lethal Dose (Oral). Report number 60118. Molnar Laboratories, Lodi, NJ, U. S.

Other

Last changed: July 26, 2000

Order number for sorting: 37

Remarks:

5.4 REPEATED DOSE TOXICITY

Test Substance

Identity:	*N*,*N*-Bis(2-hydroxyethyl) lauramide (CAS RN 120-40-1; Dodecanamide, N,N-bis(2-hydroxyethyl)-)
Purity:	92.36%
Remarks:	

Method

Method/guideline followed:	Not stated
Test type:	Oral
GLP:	Not stated
Year:	1967
Species:	Rat
Strain:	SPF
Route of administration:	Oral (feed)
Duration of test:	90 days
Doses/concentration levels:	0.1, 0.5, 1.0 and 2.0%
Sex:	Male and female
Exposure period:	90 days
Frequency of treatment:	24 hours/day, 7 days/week
Control group and treatment:	Yes (concurrent)
Postexposure observation period:	None
Statistical methods:	Not stated
Remarks:	Groups of 15 male and 15 female weanling rats with mean body weights between 106 and 123 grams were fed diets containing 2.0, 1.0, 0.5, 0.1 and 0.0% of the test substance for 90 days *ad libitum*. Examinations conducted at termination included: hematology, urinalysis, liver and kidney function tests, gross necropsy (including smear of femoral marrow) and histology. Additionally, a palatability test was conducted in which pairs of male rats were allowed access to stock diet and to diet containing either one of the four dietary test levels of the test substance. The consumption of both diets was recorded for a period of eight days.

Results

NOAEL (NOEL)	NOEL = 0.1% which corresponds to 50 mg/kg/day
LOAEL (LOEL)	Not stated
Actual dose received:	Not stated
Toxic response/effects:	Described below
Statistical results:	Not stated

Remarks: No rats died as a result of being treated with the test substance. Two males treated with diet containing 1.0% test substance were euthanized on Days 23 and 58 because of weight loss and respiratory distress. Extensive lung abscess formation was seen at autopsy and bronchopneumonia was confirmed histologically. Growth was inhibited significantly in males and females at and above the 0.5% dietary concentration. Food intake was reduced at all dietary levels except 0.1%, and was attributed to an effect of the test substance on palatability of the diet. The rats in the palatability study showed exclusive preference to the control feed than the treated feed, virtually no test diet was consumed at any dietary levels incorporated. Hematological examination revealed statistically significant reductions in hemoglobin levels and red cell counts in females at the 2.0 and 1.0% dietary concentration and in hemoglobin levels in males at the 2.0% level. Examination of the femoral bone marrow smears showed not deviation from normality. Serum chemistry revealed significantly high serum levels of glutamic-oxaloacetic transaminase in females at the 0.5% level and higher, but only at the 0.5% level in males. Urinalysis was comparable across all groups for males and females. Gross examinations were unremarkable. Statistically significant increases in relative kidney weight in all test groups except at 0.1% in females and at 2.0 and 1.0% in males; and increases in relative liver weight in females at 2.0 and 1.0% were seen. These were attributed to the decreases in body weight. Types and incidence of pathological lesions seen histologically were comparable in control and test groups. Gonads were examined histologically, thus this study meets SIDS requirements for a reproductive screen.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2A

Remarks: Reliable with restrictions; acceptable, well-documented publication which meets basic scientific principles.

References

Gaunt, I. F., M. Farmer, P. Grasso and S. D. Gangolli. 1967. Short-term Feeding Study of Lauric Diethanolamide in Rats. Fd. Cosmet. Toxicol. (5)497 - 503.

Other

Last changed: July 24, 2000
Order number for sorting: 47
Remarks:

5.4 REPEATED DOSE TOXICITY

Test Substance

Identity:	Amides, coco, N-(hydroxyethyl) (CAS RN 68140-00-1)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	OECD Method No. 407
Test type:	Oral
GLP:	Not stated
Year:	1983
Species:	Rat
Strain:	Wistar
Route of administration:	Oral gavage
Duration of test:	28 days
Doses/concentration levels:	750 (increased to 1500 after 14 days of treatment), 250 and 70 mg/kg body weight
Sex:	Male and female
Exposure period:	5 days/week for 28 days
Frequency of treatment:	One daily dose
Control group and treatment:	Yes (concurrent, treated with olive oil)
Postexposure observation period:	Not stated
Statistical methods:	Not stated
Remarks:	Ten male and 10 female rats were used on study. The test substance was administered in the vehicle, olive oil, at doses of 750, 250 and 70 mg/kg body weight per day for 14 days. After 14 days the dose in the 750 mg/kg body weight test group was increased to 1500 mg/kg body weight per day. Recovery groups consisting of five males and five females per dose level were used to determine the reversibility of possible compound related findings. The compatibility of the test substance was evaluated after 28 days of treatment.

Results

NOAEL (NOEL)	NOAEL > 750 mg/kg/day body weight
LOAEL (LOEL)	Not stated
Actual dose received:	Approximately 750 (increased to 1500 after 14 days of treatment), 250 and 70 mg/kg body weight
Toxic response/effects:	Described below
Statistical results:	Not stated
Remarks:	None of the rats died. Body weight gain and total increase in body weight did not differ from control values and no

significant compound-related gross pathology or tissue damage was noted. Biochemical parameters did not show any signs of irregulations. Slight alterations of phosphate in the highest group were noted and regarded as dose/compound -related but not as a critical effect. Gonads were examined histologically, thus this study meets the SIDS requirements for a reproductive screen.

Conclusions

Remarks: At the highest feasible dose, 750 mg/kg, daily for 28 days, no lethal dose was attained (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2B

Remarks: Reliable with restrictions; basic data given, comparable to guidelines/standards.

References

Sterzel, W. and T. Broschard. Evaluation of Repeated Dose Oral Toxicity. 1983. Report number TBD 830034. Henkel KGaA, Duesseldorf, Germany.

Other

Last changed: July 25, 2000

Order number for sorting: 122

Remarks:

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Crodamide SR (Stearamide) (CAS RN 124-26-5)
Purity:	97% minimum
Remarks:	

Method

Method/guideline followed:	OECD Method No. 471 *Salmonella typhimurium* Reverse Mutation Assay
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Yes
Year:	1989
Species/Strain:	*Salmonella typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of Sprague-Dawley derived, Aroclor 1254-induced rats; 0.5 ml of liver homogenate S-9 mix used
Concentrations tested:	50, 150, 500, 1500 and 5000 µg/plate
Statistical methods:	None
Remarks:	A dose range-finding study was conducted at dose levels of 5, 50, 500 and 5000 µg/plate prior to the bacterial mutation assay. Two independent mutation tests were performed. *Salmonella typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100 with and without rat metabolic activation, were treated with the test substance at concentrations of 50, 150, 500, 1500 and 5000 µg of sample per plate. The test substance was prepared with the solvent, ethanol. Ethanol was also used as the negative control. The following four positive controls were included: 2-aminoanthracene for all tester strains in the presence of metabolic activation (at dose levels of 0.5 – 2.0 µg/plate); and in the absence of metabolic activation N-ethyl-N'nitro-N-nitrosoguanidine (at 3 and 5 µg/plate with TA 100 and TA 1535, respectively), 9-aminoacridine (at 80 µg/plate with TA 1537) and 2-nitrofluorene (at 1.0 and 2.0 µg/plate with TA 98 and TA 1538). The criteria for a positive response were: if treatment with the test substance produced an increase in revertant colony numbers of at least twice the concurrent solvent controls, with some evidence of a positive dose-

relationship, in two separate experiments, with any bacterial strain either in the presence or absence of S-9 mix, it was considered to show evidence of mutagenic activity.

Results

Result:	No substantial increases in revertant colony numbers of any of the tester strains were observed following treatment at any dose level, either in the presence or absence of metabolic activation. No evidence of mutagenic activity was seen at any dose level of the test substance in either mutation test. Therefore, when tested at dose levels up to 5000 µg/plate in ethanol, the test substance was not mutagenic in this bacterial test system.
Cytotoxic concentration:	None with and without metabolic activation
Genotoxic effects:	Negative with and without metabolic activation
Statistical results:	None
Remarks:	A precipitate was observed in the first mutation assay at dose levels of 500 µg/plate and above, and at 1500 µg/plate and above in the repeat assay both with and without metabolic activation.

Conclusions

Remarks:	It is concluded that, when tested at dose levels up to 5000 µg/plate in ethanol, Stearamide was not mutagenic in this bacterial test system (author of the report). The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Jones, E., P., G. S. Cook, R. A. Gant and J. Kitching. 1990. Crodamide SR (Stearamide): Bacterial Mutation Assay. Report number CDA 58B/891762. Huntingdon Research Centre Ltd., Huntingdon, Cambridgeshire, UK.

Other

Last changed:	July 3, 2001
Order number for sorting:	57a
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Crodamide OR (Oleamide) (CAS RN 301-02-0)
Purity:	97% minimum
Remarks:	

Method

Method/guideline followed:	OECD Method No. 471 *Salmonella typhimurium* Reverse Mutation Assay
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Yes
Year:	1989
Species/Strain:	*Salmonella typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of Sprague-Dawley derived, Aroclor 1254-induced rats
Concentrations tested:	50, 150, 500, 1500 and 5000 µg/plate
Statistical methods:	None
Remarks:	A dose range-finding study was conducted at dose levels of 5, 50, 500 and 5000 µg/plate prior to the bacterial mutation assay. Two independent mutation tests were performed. *Salmonella typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100 with and without metabolic activation, were treated with the test substance at concentrations of 50, 150, 500, 1500 and 5000 µg of sample per plate. The test substance was prepared with the solvent, ethanol. Ethanol also was used as the negative control. The following four positive controls were included in each test: 2-aminoanthracene for all tester strains in the presence of metabolic activation (at dose levels of 0.5 – 2.0 µg/plate); and in the absence of metabolic activation N-ethyl-N'nitro-N-nitrosoguanidine (at 3 and 5 µg/plate with TA 100 and TA 1535, respectively), 9-aminoacridine (at 80 µg/plate with TA 1537) and 2-nitrofluorene (at 1.0 and 2.0 µg/plate with TA 98 and TA 1538). The mutagenic activity of the test substance was assessed by applying the following criteria: if treatment with the test substance produced an increase in revertant colony numbers of at least twice the concurrent solvent controls, with some evidence of a positive dose-relationship, in two separate experiments, with any

bacterial strain either in the presence or absence of S-9 mix, it was considered to show evidence of mutagenic activity.

Results

Result:	No substantial increases in revertant colony numbers of any of the tester strains were observed following treatment at any dose level, either in the presence or absence of metabolic activation. No evidence of mutagenic activity was seen at any dose level of the test substance in either mutation test. Therefore, when tested at dose levels up to 5000 µg/plate in ethanol, the test substance was not mutagenic in this bacterial test system.
Cytotoxic concentration:	None with and without metabolic activation
Genotoxic effects:	Negative with and without metabolic activation
Statistical results:	None
Remarks:	A precipitate was observed in the mutation assay with and without metabolic activation at dose levels of 1500 and/or 5000 µg/plate.

Conclusions

Remarks:	It is concluded that, when tested at dose levels up to 5000 µg/plate in ethanol, oleamide was not mutagenic in this bacterial test system (author of report). The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Jones, E., P. G. S. Cook, R. A. Gant and J. Kitching. 1990. Crodamide OR (Oleamide): Bacterial Mutation Assay. Report number CDA 58C/891778. Huntingdon Research Centre Ltd., Huntingdon, Cambridgeshire, UK.

Other

Last changed:	July 3, 2001
Order number for sorting:	76
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Erucamide (CAS RN 112-84-5)
Purity:	97%
Remarks:	

Method

Method/guideline followed:	OECD Method No. 471, *Salmonella typhimurium* Reverse Mutation Test
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Yes
Year:	1989
Species/Strain:	*Salmonella typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of Arochlor 1254-induced rats. S-9 mix was prepared at the laboratory.
Concentrations tested:	5000, 1500, 500, 150 and 50 µg per plate
Statistical methods:	None performed
Remarks:	Test substance was diluted in tetrahydrofuran, which was also used as the negative control.

Results

Result:	No substantial increase in revertant colony numbers of any of the test strains were observed following treatment with Erucamide at any dose level, either in the presence or absence of S-9 mix. The test substance showed no evidence of mutagenic activity when tested in this bacterial system.
Cytotoxic concentration:	Not stated
Genotoxic effects:	Negative with and without metabolic activation
Statistical results:	None
Remarks:	

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Jones, E., P. G. S. Cook, R. A. Gant and J. Kitching. 1990. Crodamide ER (Erucamide): Bacterial Mutation Assay. Report number CDA 58A/891761. Huntingdon Research Centre Ltd., Cambridgeshire, UK.

Other

Last changed: July 24, 2000
Order number for sorting: 38
Remarks:

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Lauryl ethanolamide (CAS RN 142-78-9; Dodecanamide, N-(2-hydroxyethyl)-)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Not stated
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Yes
Year:	1987
Species/Strain:	*Salmonella typhimurium* strains TA 98, TA 100, TA 1535, and TA 1537
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of Arochlor 1254-induced male Sprague-Dawley rats and male Syrian hamsters
Concentrations tested:	3.3, 10, 33, 100, 333, 1000, 3333 µg per plate
Statistical methods:	None performed
Remarks:	The preincubation assay was used. Dimethyl sulfoxide was the solvent used and also was used as the negative control. The S-9 fractions of Aroclor 1245-induced, male Sprague-Dawley rat and male Syrian hamster livers were prepared at the testing facility. The S-9 mixes were prepared immediately before use and contained 10% S-9. The doses were tested in triplicate and an independent repeat was conducted 1 week after the initial test. The 3.3 µg/plate dose was only tested with the TA1537 tester strain without activation. The 10 µg/plate level was only tested with the TA100 and TA1537 tester strains without metabolic activation.

Results

Result:	Precipitate was present at 1000 and 3333 µg/plate with all tester strains.
Cytotoxic concentration:	Complete clearing of the background lawn was observed at 333 µg/plate with the TA1537 tester strain without metabolic activation.
Genotoxic effects:	Negative with and without activation
Statistical results:	None
Remarks:	

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Reliable with restrictions; basic data given, comparable to guidelines/standards.

References

Zeiger, E., B. Anderson, S. Haworth, T. Lawlor, K. Mortelmans and W. Speck. 1987. *Salmonella* Mutagenicity Tests: III. Results From the Testing of 255 Chemicals. Journal of the Environmental Mutagen Society. 9(9):1 - 110.

Other

Last changed:	August 14, 2000
Order number for sorting:	58
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	*N*,*N*-Bis(2-hydroxyethyl) lauramide (CAS RN 120-40-1; Dodecanamide, N,N-bis(2-hydroxyethyl)-)
Purity:	93.9%
Remarks:	

Method

Method/guideline followed:	Not stated
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Not stated
Year:	1980
Species/Strain:	*Salmonella typhimurium* strains TA 98 and TA 100
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of rats pretreated with polychlorinated biphenyl
Concentrations tested:	1000, 200, 100, 50 and 10 µg per plate
Statistical methods:	None performed
Remarks:	

Results

Result:	The test substance did not induce reverse mutations in the tested strains of *Salmonella typhimurium* in the presence or absence of S-9 activation.
Cytotoxic concentration:	Not stated
Genotoxic effects:	Negative with and without activation
Statistical results:	None
Remarks:	

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions; acceptable, well-documented publication which meets basic scientific principles.

References

Inoue, K. and T. Sunakawa. 1980. Studies of *In vitro* Cell Transformation and Mutagenicity by Surfactants and Other Compounds. Fd. Cosmet. Toxicol. 18:289 - 296.

Other

Last changed:	July 25, 2000
Order number for sorting:	49a
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Amides, coco, N-(hydroxyethyl) (CAS RN 68140-00-1)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	OECD Method No. 471 (May 1983) *Salmonella typhimurium* Reverse Mutation Test
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Not stated
Year:	1981
Species/Strain:	*Salmonella typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of Arochlor 1254-induced rats. S-9 mix prepared in-house.
Concentrations tested:	2500, 500, 100, 20 and 4 µg per plate
Statistical methods:	None performed
Remarks:	

Results

Result:	The test substance did not induce reverse mutations in the tested strains of *Salmonella typhimurium* in the presence or absence of S-9 activation.
Cytotoxic concentration:	Not stated
Genotoxic effects:	Negative with and without activation
Statistical results:	None
Remarks:	

Conclusions

Remarks:	When tested at dose levels up to 2500 µg/plate, Amides, coco, N-(hydroxyethyl) was not mutagenic in this bacterial test system (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Reliable without restriction; basic data given, comparable to guidelines/ standards.

References

Sterzel, W. and T. Broschard. 1981. Evaluation of Mutagenicity. Report number TBD 810088. Henkel KGaA, Duesseldorf, Germany.

Other

Last changed: August 7, 2000
Order number for sorting: 124a
Remarks:

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Amides, C12-18, N,N-bis(hydroxyethyl) (CAS RN 68155-06-6) Compositionally equivalent to CAS RN 68603-42-9
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	OECD Method No. 471 (May 1983) *Salmonella typhimurium* Reverse Mutation Test
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Yes
Year:	1979
Species/Strain:	*Salmonella typhimurium* strains TA 100, TA 1535, TA 1537, TA 1538 and TA 98
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of male rats pretreated with Arochlor 1254
Concentrations tested:	4, 20, 100, 500 and 2500 µg per plate
Statistical methods:	None performed
Remarks:	Solutions of the test substance were freshly made up in acetone just before use.

Results

Result:	The test substance did not induce reverse mutations in the tested strains of *Salmonella typhimurium* in the presence or absence of S-9 activation.
Cytotoxic concentration:	Not stated
Genotoxic effects:	Negative with and without activation
Statistical results:	None
Remarks:	

Conclusions

Remarks:	The test substance is considered not to be mutagenic in this bacterial mutagenicity test *in vitro* (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; report lacks detail.

References

Sterzel, W. and T. Broschard. 1979. Evaluation of Mutagenicity. Report number TBD 790040. Henkel KGaA, Duesseldorf, Germany.

Other

Last changed:	July 26, 2000
Order number for sorting:	146
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Ethylenebisoctadecanamide (CAS RN 110-30-5; Octadecanamide, N,N'-ethylenebis)
Purity:	99%
Remarks:	

Method

Method/guideline followed:	Techniques described in: Ames, B. N., J. McCann and E. Yamasaki. Methods for detecting carcinogens and mutagens with the *Salmonella*/mammalian microsome mutagenicity test. Mutat. Res. 31:347 - 64.
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	not stated
Year:	1985
Species/Strain:	*Salmonella typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100; *Escherichia coli* stain WP2uvrA
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of Sprague-Dawley rats, pretreated with polychlorinated biphenyl. The S-9 mix contained 0.1 ml of S9/ml
Concentrations tested:	1, 5, 10, 50, 100, 500, 1000 and 5000 µg per plate
Statistical methods:	None performed
Remarks:	The mutagenicity was tested by the preincubation method with S9 mix, which was slightly modified from the Ames test. When *E. coli* instead of *S. typhimurium* was used, histidine and biotin in the top agar were replaced by tryptophan at the same concentration. All tests were performed in duplicate and 7 substances were used as positive controls. DMSO was used as the solvent. A contamination test was carried out in each experiment and the background bacterial lawn was checked routinely using a dissected microscope.

Results

Result:	No mutagenic activity was observed following treatment with the test substance at any dose level, either in the presence or absence of S-9 activation.
Cytotoxic concentration:	None
Genotoxic effects:	Negative with and without activation
Statistical results:	None
Remarks:	

Conclusions

Remarks:	The test substance did not exhibit genetic activity in these assays and was not mutagenic under the test conditions according to the study criteria (author of the article). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions; acceptable, well-documented publication which meets basic scientific principles.

References

Shimizu, H., U. Suzuki, N. Takemura, S. Goto and H. Matsushita. 1985. The Results of Microbial Mutation Test for Forty-three Industrial Chemicals. Jpn. J. Ind. Health 27:400 - 419.

Other

Last changed:	July 25, 2000
Order number for sorting:	26
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	4-(1-oxooctadecenyl)-1-piperazine ethanamine (CAS RN 71820-35-4; Fatty acids, tall-oil, low boiling, reaction products with 1-piperzineethanamine)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Techniques described in: Ames, B. N., J. McCann and E. Yamasaki. Methods for detecting carcinogens and mutagens with the *Salmonella*/mammalian microsome mutagenicity test. Mutat. Res. 31:347 - 364.
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Yes
Year:	1983
Species/Strain:	*Salmonella typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of Arochlor 1254-induced rats. S-9 mix prepared in-house.
Concentrations tested:	50, 15, 5, 1.5 and 0.5 µg per plate
Statistical methods:	None performed
Remarks:	A dose-range finding test was performed with the dose levels of 5000, 500, 50 and 5 µg per plate using methanol and dimethylsulphoxide solvents.

Results

Result:	The results of the range-finding tests indicated that dimethylsulphoxide was a more suitable solvent in the main mutation study. Also, the test substance was toxic towards the tester strains at the higher dose levels; therefore, 50 µg per plate was chosen as the top dose. In the main study, no substantial increases in the revertant colony numbers of any of the five strains were observed following treatment with the test substance at any dose level, either in the presence or absence of S-9 activation.
Cytotoxic concentration:	500 µg per plate
Genotoxic effects:	Negative with and without activation
Statistical results:	None
Remarks:	

Conclusions

Remarks:	There was no clear evidence of mutagenic potential of this test substance in this bacterial test system at dose levels up to 50 µg/plate (author of the article). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1B
Remarks:	Reliable without restriction; comparable to guideline study.

References

Richold, M., E. Jones and L. A. Fenner. 1983. Ames Metabolic Activation Test to Assess the Potential Mutagenic Effect of [CAS RN 71820-35-4]. Huntingdon Research Centre, Cambridgeshire, UK.

Other

Last changed:	July 25, 2000
Order number for sorting:	154
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	*Sanitized report – chemical name not stated.* (CAS RN 71820-35-4; Fatty acids, tall-oil, low boiling, reaction products with 1-piperzineethanamine)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Not stated
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Yes
Year:	1985
Species/Strain:	*Salmonella typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of Aroclor 1254-induced rats
Concentrations tested:	Dose range-finding test: 5000, 500, 50 and 5 µg/plate Mutation test: 150, 50, 15, 5 and 1.5 µg/plate
Statistical methods:	None performed
Remarks:	Dimethylsulphoxide was the solvent used in this study and was also used as the negative control. Test was conducted with and without metabolic activation with S-9 mix. Each dose level was run in triplicate with an independent repeat.

Results

Result:	Negative
Cytotoxic concentration:	500 µg/plate
Genotoxic effects:	Negative with and without activation
Statistical results:	None
Remarks:	

Conclusions

Remarks:	No evidence of mutagenic potential of the test substance was obtained in this bacterial test system at the dose levels used (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions; acceptable, well-documented publication/study report which meets basic scientific principles.

References

Richold, M., E. Jones, and L. A. Fenner. 1985. Ames Metabolic Activation Test to Assess the Potential Mutagenic Effect of [CAS RN 71820-35-4]. Huntingdon Research Centre, Cambridgeshire, UK.

Other

Last changed:	July 27, 2000
Order number for sorting:	155
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	EH&S 751(CAS RN 68910-87-2; Fatty acids, tall-oil, reaction products with polyalkylenepolyamines, dodecylbenzenesulfonates)
Purity:	100%
Remarks:	

Method

Method/guideline followed:	OECD 471 and 472
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Yes
Year:	1996
Species/Strain:	*Salmonella typhimurium* strains TA 98, TA 100, TA 1535 and TA 1537 and *E. coli* strain WP2 uvrA
Metabolic activation:	With and without Aroclor-induced rat S-9 activation
Concentrations tested:	3.3 to 3333 µg per plate for all *s. typh*. strains without metabolic activation 10 to 3333 µg per plate for all *s. typh*. strains with metabolic activation 10 to 5000 µg per plate for the E. coli strain with and without metabolic activation.
Statistical methods:	None used.
Remarks:	The Aroclor 1254-induced rat liver S-9 was prepared at the laboratory facility and frozen. The S-9 mix was prepared immediately before use. Ethanol was used as the solvent. A preliminary toxicity assay was performed with and without S-9 activation with a maximum dose level of 5000 µg/plate. In the mutagenicity assay, a minimum of five dose levels of the test article along with the appropriate vehicle and positive controls were plated both in the presence and absence of rat liver S-9 activation. All dose levels of test article, vehicle controls and positive controls were plated in triplicate using the plate incorporation assay. An independent repeat assay was performed.

Results

Result:	Preliminary Toxicity Assay: Toxicity was generally observed at 667 µg/plate with *Salmonella* only. Mutagenicity Assay: Precipitate was observed at ≥ 333 to ≥ 1000 µg/plate and toxicity was observed at ≥ 333 to ≥ 1000 µg/plate with *Salmonella*. No positive responses were observed with any of the tester strains in the presence

	and absence of S-9 activation in both the initial assay and the independent repeat assay.
Cytotoxic concentration:	≥ 333 µg/plate of *Salmonella* > 5000 µg/plate of *E. Coli*
Genotoxic effects:	Negative with and without activation
Statistical results:	None
Remarks:	

Conclusions

Remarks:	Under the conditions of this study, the test article, EH&S 751 was negative in the bacterial reverse mutation assay (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Wagner, V. O. and K. E. Burnett. Bacterial Reverse Mutation Assay with an Independent Repeat Assay. 1996. Report number EHS-751. Microbiological Associates, Inc., Rockville, MD, U. S.

Other

Last changed:	July 25, 2000
Order number for sorting:	162
Remarks:	

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Test Substance

Identity:	Comperlan KD (CAS RN 68603-42-9; Amides, coco, N, N-bis(hydroxyethyl))
Purity:	90 - 95% (Amides, coco, N,N-bis (hydroxyethyl))
Remarks:	

Method

Method/guideline followed:	OECD 414
GLP:	Yes
Year:	1994
Species:	Rat
Strain:	Sprague-Dawley CD
Route of administration:	Oral gavage
Doses/concentration levels:	0, 100, 300 and 1000 mg/kg/day
Sex:	Female
Exposure period:	Days 6 - 15 of gestation
Frequency of treatment:	7 days/week
Control group and treatment:	Yes (concurrent, treated with arachis oil, DAB 9)
Duration of test:	Days 0 - 20 of gestation
Statistical methods:	If normal distribution, Dunnett-Test comparing treated groups to control. The Steel-Test was applied when the data could not be assumed to follow normal distribution. Fisher's Exact Test for 2 x 2 tables was applied if the variables could be dichotomized without loss of information (Bonferroni-Holm-corrected).
Remarks:	Females were mated at the supplier and received at the testing facility on day 0 of gestation. Dose volume was 5 ml/kg body weight, adjusted for body weighed on day 6 of gestation. Animals were observed at least twice daily for signs of reaction to treatment and/or symptoms of illness. Body weights were recorded on day 0, 6, 16 and 20 of gestation. Females were sacrificed by on overdose of ether on day 20 of gestation. The uterus was weighed and the fetuses were removed by caesarean section. Corpora lutea were counted and the number and distribution of intrauterine implantations were classified as live or dead fetuses, late intrauterine deaths (resorptions), or early intrauterine deaths (resorption sites). Intrauterine deaths were classified on the basis of the presence (late) or absence (early) of fetal or decidual tissue in addition to placental tissue. Live fetuses were weighed individually including placenta and examined for external abnormalities. One half of the fetuses for each litter were

fixed in Bouin's solution to examine the viscera and brain by Wilson's slicing technique. After examination these tissues were discarded. The remaining fetuses were processed (alizarin red staining), examined for skeletal abnormalities and retained.

Results

Maternal toxicity NOAEL: 1000 mg/kg/day

Developmental toxicity NOEAL: 1000 mg/kg/day

Actual dose received: 0, 100, 300 and 1000 mg/kg/day

Maternal data: No deaths occurred in any dams in the control or treated groups. Compound-related symptoms were observed in all treatment groups as salivation (severe in the 1000 mg/kg/day group) and propulsion of the head. Body weight, body weight gains and corrected body weight gains were comparable across all groups. There were no significant macroscopic findings in any of the control or treated animals.

Fetal data: Litter parameters:

Post-implantation loss and total embryonic deaths were statistically significantly increased in all treated groups compared to the control group. These findings were considered incidental because in each group there was one single female with a high incidence of embryonic deaths and the incidence of post weight loss was not dose-dependent. The sex ratio of the fetuses was not affected by the treatment with the test substance.

Body weights:

There were no significant differences in the body weights of live fetuses (on a litter or individual basis) between the treated and control groups

External examinations:

There were no external macroscopic findings noted in any fetus that were considered to be an effect of the treatment with the test article.

Visceral examinations of the preserved fetuses did not reveal any treatment-related abnormalities.

Skeletal examinations

Statistically significant retardation in ossification was observed in the 300 and 1000 mg/kg/day groups compared to the controls. The incidence of two sternebrae unossified was significantly increased in the 300 and 1000 mg/kg/day groups compared to the control group. The incidence of incomplete ossification of the skull bones was also significantly increased in the 1000 mg/kg/day group

compared to the control group but was essentially due to two dams, which had a total of 10 incomplete ossified skull bones of the 17 observed for this group. The skeletal retardation effects were considered to be incidental because the values were within the normal range of variation for this strain.

Statistical results: Described above
Remarks:

Conclusions

Remarks: The results of this study showed that repeated oral administration of COMPERLAN KD to pregnant rats on day 6 through 15 of gestation, caused no symptoms of cumulative toxicity up to a dose level of 1000 mg/kg/day. With the exception of salivation and propulsion of the head during the dose administration, there were no treatment-related effects. Also, COMPERLAN KD does not reveal any embryotoxic or teratogenic potential at dose levels up to 1000 mg/kg/day (author of the report).
The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1A
Remarks: Reliable without restrictions; guideline study.

References

Pittermann, W. 1994. Embryotoxicity Study (Including Teratogenicity) in the Rat (Segment II). Report number RT 920403. Henkel KGaA, Duesseldorf, Germany.

Other

Last changed: July 26, 2000
Order number for sorting: 147
Remarks:

Robust Summaries
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September 16, 2004

Appendix 2

3.5 BIODEGRADATION

4.2 TOXICITY TO AQUATIC INVERTEBRATES

5.1.1 ACUTE ORAL TOXICITY

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY *IN VITRO*

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

3.5 BIODEGRADATION

Test Substance

Identity: SURFAM P-12B (CAS RN 68122-86-1; Imidazolium compounds, 4,5-dihydro-1-methyl-2-nortallow alkyl-1-(2-tallow amidoethyl) Me sulfate)

Purity: Not stated

Remarks:

Method

Method/Guideline followed: Not stated

Test type: Biochemical oxygen demand

GLP: Not stated

Year: 1988

Contact time: 20 days

Inoculum: Secondary effluent from both the Michigan Division's 437 Wastewater Treatment Plant and the City of Midland Wastewater Treatment Plant.

Remarks: Two different bacterial seed sources were used at a concentration of 45 ml of effluent per liter of seed solution. The seed activity was checked by running a 5-day BOD test on a standard solution of glucose-glutamic acid.

Results

Degradation:

	Municipal Seed		Industrial Seed	
Day	**BOD (p/p)**	**BOD/TOD (%)**	**BOD (p/p)**	**BOD/TOD (%)**
5	0.04	5	0.03	4
10	0.04	5	0.03	4
20	0.05	5	0.03	4

Results: The test substance consumed little oxygen in the BOD test. The fact that the BOD is the same after 5, 10 and 20 days of incubation indicates that a minor component of the sample (probably acrylic acid) is degraded in the first five days while the Surfam component itself does not degrade.

Kinetic: None stated

Breakdown products: None stated

Remarks: The test substance would not be expected to significantly degrade in a conventional biological wastewater treatment plant.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; limited details available.

References

U. S. EPA. 1988. Twenty One Reports on Four Different Chemicals with Attachments and Cover Letter Dated 081788 (Sanitized). Document number 86-880000345.

Other Available Reports

Other

Last changed:	July 3, 2001
Order number for sorting:	166b
Remarks:	

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	1-(2-hydroxyethyl)-2-heptadecenyl-2-imidazoline (EH&S 686) (CAS RN 61791-39-7; 1H-Imidazole-1-ethanol, 4,5-dihydro-, 2-nortall-oil alkyl derivs)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	U. S. EPA FIFRA 40 CFR 158, Guideline 158.490
Test type:	Static
GLP:	Yes
Year:	1994
Analytical procedures:	No
Species/Strain:	*Daphnia magna*
Test details:	Static
Statistical methods:	Computer-generated LC_{50} calculations (Stephan, C. E. 1983. Computer program for calculation of LC_{50} values. U. S. EPA. Duluth, MN, U. S. Personal communication.) using probit and moving average methods
Remarks:	The experiment measured the survival of *Daphnia magna* over a 48-hour exposure to the test and control substances. Daphnids were cultured at the laboratory in dechlorinated tap water. Daphnids were healthy prior to the test. Daphnids less than 24-hours old were exposed to five concentrations of the test substance and a dilution water control. The nominal test concentrations were: 0 (control), 1.3, 2.2, 3.6, 6.0 and 10 mg/l. Treatments were replicated twice with 10 daphnids per replicate (20 daphnids per experimental group). Test vessels were 300-ml glass beakers containing 250 ml of solution. At test initiation, daphnids were indiscriminately distributed to the test vessels; the test vessels were loosely covered and randomly assigned to a location in the testing area. A 16-hour light/8-hour dark photoperiod was provided using cool-white fluorescent lights at an intensity of 3 μEin/sec/m^2. Dissolved oxygen (DO), water pH, conductivity and temperature were measured each day in each test chamber that contained live daphnids. Dilution water was dechlorinated tap water adjusted to a hardness of 180 mg/l. The target test temperature was 20±1 °C. The number of surviving daphnids and the occurrence of sublethal effects (immobilization, loss of equilibrium, erratic swimming, loss of reflex, excitability, discoloration, or change in

behavior) were determined visually and recorded initially and after 24 and 48 hours. Effect concentrations were based on nominal concentrations.

Results

Nominal concentrations (mg/l):	0 (control), 1.3, 2.2, 3.6, 6.0 and 10
Measured concentrations (mg/l):	Not measured
Unit:	mg/l
EC_{50} (48-hour):	1.5 mg/l (95% confidence limits: 1.2 – 1.8 mg/l)
LC_{50} (48-hour):	1.7 mg/l (95% confidence limits: 1.3 – 2.0 mg/l)
NOEC (48-hour):	< 1.3 mg/l
Statistical results:	Described above
Remarks:	No deaths or abnormal effects occurred in the control group of daphnids. The percent mortality at 48 hours in the 1.3, 2.2, 3.6, 6.0 and 10 mg/l treatment groups were 35, 60, 100, 100 and 100%, respectively. Surviving daphnids in the 1.3 mg/l treatment showed no abnormal effects, while four of eight surviving daphnids in the 2.2 mg/l treatment were immobilized. The 6.0 and 10 mg/l test solutions were slightly cloudy at the start of the toxicity test. No other insoluble material was noted during the exposure period.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Ward, T. J., J. P. Magazu and R. L. Boeri. 1994. Static Acute Toxicity of EH&S 686 to the Daphnid, *Daphnia magna*. Report number 513-NA. T. R. Wilbury Laboratories, Inc., Marblehead, MA, U. S.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	106

Remarks:

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	1H-Imidazole-1-ethanamine,4,5-dihydro-,2-nortall-oil alkyl derivatives (CAS RN 68442-97-7)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	FDA 16 CFR 1500.3 – Commercial Practices
Type:	LD_{50} limit test
GLP:	Yes
Year:	1984
Species/Strain:	Sprague-Dawley Rats
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Oral gavage
Remarks:	Five young male and five young female rats (209 - 298 g) were administered a single dose of the undiluted test substance at a level of 5.0 g/kg body weight. Animals were fasted from food overnight prior to dosing. Animals were weighed prior to dosing and at termination. They were observed frequently on the day of dosing and daily thereafter for a total of 15 days. All external signs of toxicity or pharmacological effects were noted. All animals that died during the study were subjected to a gross necropsy and abnormalities were recorded.

Results

Value:	Not stated
Number of deaths:	6
Remarks:	Sixty percent of the animals (4 of 5 males and 2 of 5 females) died during the study. No gross lesions were observed during the necropsy of these animals. Eighty to 100% of the animals exhibited decreased activity, ataxia, diarrhea and salivation.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1C
Remarks:	Reliable without restrictions; guideline study.

References

Acute Oral Toxicity Study in Sprague-Dawley Rats with a Fatty Acid Imidazoline with Cover Letters Dated 10/06/84 and 10/29/84 (Sanitized). 1984. EPA document number 8EHQ-1084-05315.

Other Available Reports

Other

Last changed:	July 25, 2000
Order number for sorting:	126
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Carsosoft S-90 (CAS RN 68122-86-1; Imidazolium compounds, 4,5-dihydro-1-methyl-2-nortallow alkyl-1-(2-tallow amidoethyl) Me sulfate)
Purity:	90% active ingredient
Remarks:	

Method

Method/guideline followed:	Not stated
Type:	LD_{50} limit test
GLP:	Not stated
Year:	1978
Species/Strain:	Albino rats/Not stated
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	Not stated
Route of administration:	Oral
Remarks:	Groups of five male and five female rats (180 - 399 g) were administered a single oral dose of 5.0 g/kg test material and observed for 14 days.

Results

Value:	LD_{50} > 5 g/kg
Number of deaths:	None
Remarks:	Not a toxic material to rats under conditions of this test.

Conclusions

Remarks:	The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; data are reliable but article lacks details.

References

U. S. EPA. 1978. Primary Dermal Irritation, Dermal Corrosion & Ocular Irritation Studies in Rabbits & Acute Oral Toxicity Study in Rats on Two Chemicals with Cover Letter Dated 081288. Document I. D. number 86-880000338.

Other available reports

Other

Last changed: July 3, 2001
Order number for sorting: 164
Remarks:

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity: Miranol J2M (CAS RN 68122-86-1; Imidazolium compounds, 4,5-dihydro-1-methyl-2-nortallow alkyl-1-(2-tallow amidoethyl) Me sulfate)

Purity: Not stated

Remarks:

Method

Method/guideline followed: Not stated

Type: Acute oral

GLP: Not stated

Year: Not stated

Species/Strain: Rats/Not stated

Sex: Male and female

No. of animals per sex per dose: 5

Vehicle: None

Route of administration: Gavage

Remarks: After overnight fasting the undiluted test substance was administered in one single dose by gavage. For each dose level five males and five females were treated. On the basis of preliminary observations, 7.0, 7.5, 8.0, 8.5 and 9.0 ml of the undiluted test substance were administered per kg of body weight. After treatment the rats received stock diet and tap water *ad libitum*. After an observation period of 14 days the survivors were killed and examined grossly.

Results

Value: LD_{50} = 8.45 ml/kg body weight with 95% confidence limit of 8.79 - 8.13 ml/kg

Number of deaths:

Dose (ml/kg)	Number of Males	Number of Females	Percent Mortality
7.0	0/5	0/5	0
7.5	0/5	1/5	10
8.0	3/5	2/5	50
8.5	2/5	1/5	50
9.0	4/5	4/5	80

Remarks:	Two hours after treatment all rats showed diarrhea. The animals became sluggish, showed signs of paralysis and lost consciousness. Several died within 12 hours. The survivors looked quite healthy again after 12 hours. At the autopsy of the surviving rats at day 14, no microscopic changes were observed.

Conclusions

Remarks:	The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; limited details available

References

U. S. EPA. 1988. Twenty One Reports on Four Different Chemicals with Attachments and Cover Letter Dated 081788 (Sanitized). Document number 86-880000345.

Other available reports

Other

Last changed:	July 3, 2001
Order number for sorting:	166b-2
Remarks:	

5.4 REPEATED DOSE TOXICITY

Test Substance

Identity:	Varisoft 475 (75%) (CAS RN 68122-86-1; Imidazolium compounds, 4,5-dihydro-1-methyl-2-nortallow alkyl-1-(2-tallow amidoethyl) Me sulfate)
Purity:	76.6% in isopropyl alcohol
Remarks:	

Method

Method/guideline followed:	U. S. EPA Pesticide Assessment Guidelines, Subdivision F, Hazard Evaluation: Human and Domestic Animals (Guideline 82-2)
Test type:	Oral
GLP:	Yes
Year:	1992
Species:	Dog
Strain:	Beagle
Route of administration:	In food
Duration of test:	13 weeks
Doses/concentration levels:	4000, 12000 and 40000 ppm (142, 366 and 1322 mg/kg/day for males; 144, 632 and 1948 mg/kg/day for females
Sex:	Male and female
Exposure period:	91 to 93 days
Frequency of treatment:	Daily
Control group and treatment:	Yes, control diet
Postexposure observation period:	None
Statistical methods:	Analysis of variance, Bartlett's Test for Homogeneity of Variance, T-statistic as described by Steel and Torrie, Ostle and Dunnett's Tables with a Bonferroni correction
Remarks:	The study evaluated the subchronic oral toxicity of Varisoft 475 (75%) in a 13-week study in dogs. Four male and four female beagle dogs were offered the test substance in the diet at concentrations of 0, 4000, 12000 and 4000 ppm active ingredient for 13 weeks. Diet and water were available *ad libitum*, except prior to clinical pathology testing and necropsy, when diet and/or water were withheld overnight. Male animals weighed between 9.1 to 11.6 kg and females weighed 6.5 to 8.8 kg. Observations were conducted at least twice daily for mortality and overt toxicity. Detailed observations, body weights and food consumption were recorded weekly. Ophthalmologic examinations were performed on all animals prior to study initiation and at study termination. Physical examinations,

as well as hematological clinical chemistry and urological evaluations were conducted on all animals prior to study initiation and at monthly intervals during the study. At study termination, a thorough post-mortem examination was conducted on all dogs. A complete set of all major tissues and organs was harvested and selected organs were weight. The saved tissues were processed histologically and microscopic examination was conducted.

Results

NOAEL (NOEL)	NOEL = 4,000 ppm (143 mg/kg/day)
LOAEL (LOEL)	12,000 ppm (366 and 632 mg/kg/day for males and females, respectively)
Actual dose received:	142, 366 and 1322 mg/kg/day for males; 144, 632 and 1948 mg/kg/day for females
Toxic response/effects:	Described below
Statistical results:	Described below
Remarks:	During the 13-week treatment period, one male and one female dog administered diets containing 40,000 ppm test substance lost 1.4 and 1.1 kg of body weight, respectively. The body weight gains of all other male and female dogs administered test substance in their diet were considered to be comparable to the body weight gains of the respective control animals in this study. During the first week of the study, there was a clear reduction in food consumption, indicating an aversion to the treated diets, in both the male and female dogs administered diets containing 40,000 ppm test substance. Thereafter, there continued to be evidence of aversion to the treated diets. In males, this was evidenced by a slight reduction in food consumption in all treatment groups. In females, the aversion was evidenced by an apparent increase in food spillage, which was considered to at least partially account for the difference in actual received dosages between males and females. All dogs survived to study termination. No changes noted in physical condition or appearance were considered to be related to treatment with the test substance. At termination, body weights appeared to be reduced for males and females receiving 40,000 ppm of the test substance in the diet. However, the reduction was due to the body weight loss of the one male and one female dog noted above. Small reductions in mean values for erythrocyte, hemoglobin and hematocrit were observed in both male and female dogs in the 40,000 ppm treatment group relative to the corresponding mean control values at one or more intervals

of analysis. The differences were slight, a slight difference was also observed in the pre-study measurements, and the values were within historical control range. Therefore, the toxicological significance of the changes in hematology measurements was unclear. At all analysis intervals during the treatment period, mean cholesterol values for male and female dogs in the 40,000 ppm treatment group were reduced relative to the corresponding control group. The mean cholesterol values for the male dogs in the 12,000 ppm treatment group were also reduced relative to the corresponding controls. No treatment-related changes in urinalysis measurements were observed. No treatment-related ophthalmologic changes or clinical observations, organ weight changes, or gross necropsy observations were seen at termination. A small number of macroscopic lesions were seen in both male and female animals across dietary concentrations. These lesions were considered to be spontaneous and not related to the administration of the test article. The ratio of the weight of the pituitary gland to the body weight of males at the 12,000 ppm dietary concentration was significantly decreased relative to the control group. The ratio of the weight of the pituitary gland to the body weight of females in the 4,000 ppm dietary concentration also was significantly decreased compared to the control group. The ratio of the weight of the right adrenal gland to the brain weight of the females was significantly increased at the 4,000 ppm dietary concentration compared to the control group. These findings were not consistent, could not be correlated with microscopic findings and were considered to be either spurious or due to biological variation, and not related to the administration of the test article. A small number of non-neoplastic findings were evident in this study. Many of them occurred in single animals. Some of the more common lesions included interstitial pneumonia, parathyroid cysts, pituitary cysts, thymic atrophy, c-cell hyperplasia of the thyroid gland and mineralization of the kidneys. Multifocal mineralization of the renal medulla of the kidneys was present in both male (16/16) and female (15/16) dogs of all dietary concentrations. The above lesions are considered to be common spontaneous findings in a 13-week beagle dog study, and none of the microscopic findings were considered to be related to the administration of the test article. Reproductive organs were

examined meeting the requirements for SIDS/HPV reproductive screening.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1A
Remarks: Reliable without restriction; guideline study.

References

Evaluation of Varisoft 475 (755) in a 13-Week Dietary Toxicity Study in Dogs (Volume I-II) with Attachments and Cover letter dated 052192. U. S. EPA Document number 86-920000941. Microfiche Number OTS0536282.

Other

Last changed: July 3, 2001
Order number for sorting: 166e
Remarks:

5.4 REPEATED DOSE TOXICITY

Test Substance

Identity:	Miranol J2M (CAS RN 68122-86-1; Imidazolium compounds, 4,5-dihydro-1-methyl-2-nortallow alkyl-1-(2-tallow amidoethyl) Me sulfate)
Purity:	37% minimum active ingredient
Remarks:	

Method

Method/guideline followed:	Not stated
Type	Dietary feeding study
GLP:	Not stated
Year:	1963
Species/Strain:	Not stated
Sex:	Male and female
No. of animals per sex per dose:	10
Vehicle:	Ground Purina Laboratory Chow
Route of administration:	In feed
Remarks:	Groups of male and female rats (ten of each sex per group) were maintained for 91 days on diets containing the following test substance concentrations: 0.0, 3.0, 1.0, 0.3 or 0.03 percent (approximately 0, 2200, 730, 220 and 22 mg/kg/day). The animals were weaned twice weekly for the first 28 days and once a week thereafter. They were observed frequently for gross changes in appearance or behavior. In addition, records were kept of mortality, and food consumption was recorded for the first month. Terminal hematological values were obtained from five female rats at the 0.0, 3.0 and 1.0 percent levels. At necropsy, the animals were fasted overnight, weighed and killed by decapitation. The lungs, heart, liver, kidneys, spleen and testes were removed and weighed. Portions of each organ, as well as adrenal, pancreas, thyroid, brain, stomach, small intestine and large intestine were preserved. Samples of blood serum were obtained for the determination of urea nitrogen content and alkaline phosphatase activity. The tissues were examined microscopically. The Fisher "t" test was used in comparing the mean values obtained from the experimental groups with those of the controls; in general, probability values (p) of less than 0.05 were interpreted as indicating a significant difference.

Results

Value:	NOAEL > 2200 mg/kg/day
Number of deaths:	
Remarks:	Groups of male and female rats that received the test substance in their diets in concentrations as high as 3.0 percent for a period of 91 days showed no evidence of adverse effect that can be attributed to the inclusion of the test material. Judgment was based on general appearance and behavior, growth, mortality, food consumption, terminal hematological values, serum urea nitrogen and alkaline phosphatase determinations, final average body and organ weights, and gross and microscopic examination of the tissues. Statistically significant increases were found in the final average liver/body weight ratios of the male rats that received 3.0 percent of the test substance in their diets and the females on all the levels except 0.1 percent. The final average weights of the kidneys of the female rats on the 3.0 and 1.0 percent levels were also significantly increased. However, the average weights of the livers of both sexes of controls and the kidneys of the female controls used for comparison were lower than those usually found for untreated rats in these body weight ranges, resulting in statistical variations in the test groups of no practical importance. The statistically significant increases in the final average organ/body weight ratio of the spleens of the females that received 1.0, 0.3 or 0.03 percent Miranol J2M concentrate are not believed to be due to the inclusion of the test material in feed, since there was no increase on the top level, and noncellular changes were observed upon microscopic examination. The test substance is judged to be extremely low in repeated oral toxicity when fed as apart of the diet to male and female rats for a period of 91 days. Dietary levels of 3.0 percent and below were tolerated without evidence of adverse effects.

Conclusions

Remarks:	The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions; acceptable, well-documented study report that meets basic scientific principles.

References

U. S. EPA. 1988. Twenty One Reports on Four Different Chemicals with Attachments and Cover Letter Dated 081788 (Sanitized). Document number 86-880000345.

Other available reports

Other

Last changed:	July 3, 2001
Order number for sorting:	166b-1
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Varisoft 475 (75%) (CAS RN 68122-86-1; Imidazolium compounds, 4,5-dihydro-1-methyl-2-nortallow alkyl-1-(2-tallow amidoethyl) Me sulfate)
Purity:	75% in isopropyl alcohol
Remarks:	

Method

Method/guideline followed:	Based on the direct plate incorporation method published by Ames *et al.* (1975)
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Yes
Year:	1988
Species/Strain:	*Salmonella typhimurium* strains TA1535, TA1537, TA1538, TA98 and TA100/obtained from Dr. Bruce Ames, University of California at Berkeley, CA
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of male Sprague-Dawley derived, Aroclor 1254-induced rats
Concentrations tested:	0.05, 0.10, 0.50, 1.00, 2.00, 4.00 and 8.00 µl per plate
Statistical methods:	None
Remarks:	The test substance was prepared with the solvent, dimethylsulfoxide (DMSO). A dose range-finding test was conducted using TA100 bacterial strain and concentrations of 0.018 to 150 µl/plate without activation. Based on the results of the dose range-finding test, *Salmonella typhimurium* strains TA1535, TA1537, TA1538, TA98 and TA100 were treated with the test substance at concentrations of 0.05 to 8.00 µl of sample per plate with and without metabolic activation. The assays were conducted using three plates per dose level. An independent repeat assay was performed. Negative controls (solvent only) were assayed concurrently with the test substance, both in the presence and absence of metabolic activation. The following positive controls were included in each test: 2-anthramine (for all bacterial strains, 2.5 µg/plate) in the presence of metabolic activation; and sodium azide (TA1535 and TA100, 10 µg/plate), quinacrine mustard (TA1537, 5 µg/plate) and 2-nitrofluorene (TA1538 and TA98, 10 µg/plate) in the absence of metabolic activation.

Criteria for a positive response were:

- Strains TA1535, TA1537 and TA1538: data sets were evaluated as positive if a dose response was observed over a minimum of three test concentrations and the increase in revertants was equal to or greater than three times the solvent control value at the peak of the dose response. The solvent control value should be within the normal range for evaluating the results.
- Strains TA98 and TA100: data sets were evaluated as positive if a dose response was observed over a minimum of three test concentrations and the increase in revertants achieved a doubling of the solvent control value at the peak of the dose response. The solvent control value should be within the normal range for evaluation the results.

Results

Result:	The test substance did not exhibit genetic activity in these assays and was not mutagenic under the test conditions according to the assay criteria.
Cytotoxic concentration:	The test substance exhibited varying degrees of toxicity with all the strains at 4.0 and 8.0 µl/plate in the nonactivation and activation assays. The dose range-finding study showed decreased bacterial lawn at 2.34 µl/plate and above and an absence of the background lawn at concentrations of 18.8 µl/plate and higher.
Genotoxic effects:	Negative with and without activation
Statistical results:	
Remarks:	

Conclusions

Remarks:	The test material, Varisoft 475 (75%), did not exhibit genetic activity in any of the assays conducted in this evaluation and was not mutagenic to the *Salmonella typhimurium* indicator organism under these test conditions according to the defined evaluation criteria (author of the report). The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Sherex Chem. Co. 1989. Mutagenicity Test on Varisoft 475 (75%) in the Ames *Salmonella*/Microsome Reverse Mutation Assay with Cover Letter Dated 040689. EPA Document number 86-890000177.

Other

Last changed:	July 3, 2001
Order number for sorting:	165
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Varisoft 475 (75%) (CAS RN 68122-86-1; Imidazolium compounds, 4,5-dihydro-1-methyl-2-nortallow alkyl-1-(2-tallow amidoethyl) Me sulfate)
Purity:	75% in isopropyl alcohol
Remarks:	

Method

Method/guideline followed:	OECD guideline no. 473
Type:	Cytogenetic assay (chromosomal aberration)
System of testing:	Nonbacterial
GLP:	Yes
Year:	1988
Species/Strain:	Chinese hamster ovary (CHO-WBL); originally obtained from the laboratory of Dr. S. Wolff, University of California, San Francisco, CA
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of male Sprague-Dawley derived, Aroclor 1254-induced rats
Concentrations tested:	3.74 to 74.8 µg/ml without activation 15.0 to 199 µg/ml with activation
Statistical methods:	Fisher's Exact Test
Remarks:	The test substance was suspended in deionized water at a stock concentration of 49.6 mg/ml. A 1:10 dilution of this stock solution and serial dilutions of this dilution were used in the range-finding assays for testing concentrations of 0.165 to 4960 µg/ml in a half-log series. Range-finding and chromosomal aberration assays were tested with and without metabolic activation. Because no cell cycle delay was evident at the doses with viable metaphase cells in either range-finding assay, a ten-hour harvest was selected for the aberrations assays. Duplicate cultures of CHO cells were used for all test material concentrations. Single cultures were used for the negative control, solvent control and at each of two doses of the positive control. Solvent controls were cultures containing the solvent, deionized water, at the same concentration used in test cultures. The positive controls used in the assays were mitomycin C (0.25 and 0.50 µg/ml for the range-finding assays and 0.5 and 1.0 µg/ml for the chromosomal aberrations assays) for the nonactivation series and cyclophosphamid (12.5 and 20.0 µg/ml for the range-finding assays and 25.0 and 50.0 µg/ml for the chromosomal aberrations assays) in the

metabolic activation series. Chromosomal aberrations were analyzed from the four highest doses from which results could be obtained and from only one of the positive control doses. The following factors were taken into account in the evaluation of the chromosomal aberrations data:

- The overall chromosomal aberration frequencies;
- The percentage of cells with any aberrations;
- The percentage of cells with more than one aberration; and
- Any evidence for increasing amounts of damage with increasing dose, i.e. a positive dose response; The estimated number of breaks involved in the production of the different types of aberrations that were observed, i.e. complex aberrations may have more significance than simple breaks.

Deviations from OECD Guidelines: The highest dose used in this assay was one that allowed the collection of a suitable number of mitotic cells (maximum tolerated dose). The guideline suggests that the high dose used should suppress mitotic activity by about 50%. Because the laboratory collects purely mitotic cells, they do not carry out a mitotic index estimation as suggested in the guidelines. Suppression of mitotic activity is estimated from the test for cell cycle delay and from observations of cell monolayers before fixation.

Results

Result: No significant increase in chromosomally aberrant cells was observed at any of the concentrations analyzed. The test substance is considered negative for inducing chromosomal aberrations in CHO cells under both nonactivation and activation conditions of this assay.

Cytotoxic concentration: Complete cellular toxicity was observed at 165, 496, 1650 and 4960 µg/ml in the nonactivation range-finding assay and at 496, 1650 and 4960 µg/ml in the range-finding assay with metabolic activation. In the chromosomal aberrations assay without metabolic activation, signs of toxicity (unhealthy cell monolayer, reductions in the cell monolayer confluence and/or reductions in visible mitotic cells) were observed at 37.4 µg/ml. In the chromosomal aberrations assay with metabolic activation, signs of toxicity (floating dead cells, floating debris, unhealthy cell monolayer, reductions in visible mitotic cells and/or reductions in the cell monolayer confluence) were observed at 49.9 µg/ml and above.

Genotoxic effects:	Negative with and without metabolic activation
Statistical results:	Results of test substance groups not significantly different from solvent control group.
Remarks:	

Conclusions

Remarks:	The test article, Varisoft 475 (75%), is considered negative for inducing chromosomal aberrations in Chinese hamster ovary cells under both nonactivation and activation conditions of this assay (author of the report). The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Sherex Chem. Co. 1989. Mutagenicity Test on Varisoft 475 (75%) in an *In Vitro* Cytogenetic Assay Measuring Chromosomal Aberration Frequencies in CHO Cells with Cover Letter Dated 933189. EPA Document number 86-890000165.

Other

Last changed:	July 3, 2001
Order number for sorting:	166
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Varisoft 475 (75%) (CAS RN 68122-86-1; Imidazolium compounds, 4,5-dihydro-1-methyl-2-nortallow alkyl-1-(2-tallow amidoethyl) Me sulfate)
Purity:	75% in isopropyl alcohol
Remarks:	

Method

Method/guideline followed:	EPA FIFRA Good laboratory Practice Standards as set forth in Title 40 of the U. S. Code of federal Regulations Part 160
Type:	Unscheduled DNA synthesis
System of testing:	Nonbacterial
GLP:	Yes
Year:	1989
Species/Strain:	Hepatocytes obtained from adult male Fischer 344 rats, purchased from Charles River Breeding Laboratories, Inc. (CDF(F344)/CrlBR)
Metabolic activation:	Not applicable
Concentrations tested:	See below
Statistical methods:	Fisher's Exact Test
Remarks:	A solution of test substance in DMSO was serially diluted with DMSO and each stock was diluted 1:100 into medium (WMEI) to obtain the final desired concentrations of test material. Fresh preparations of test material in the vehicle were used for each trial. Treatments were initiated by replacing the medium on the cell cultures with WMEI containing the test material at the desired concentrations and 5 µCi/ml ^{3}H-thymidine (20 Ci/mmole). In the two trials described in this report, twelve to sixteen doses were initiated and six concentrations from each trial were chosen for analysis of nuclear labeling, starting with the highest dose that resulted in a sufficient number of survivors with intact morphologies and proceeding to successively lower doses (Assay 1 = 0.25, 0.50, 1.00, 2.00, 3.00 and 4.00 µg/ml; Assay 2 = 0.50, 1.00, 2.00, 3.00, 4.00 and 5.00 µg/ml).

Results

Result:	In the *in vitro* rat primary hepatocyte unscheduled DNA synthesis (UDS) assay, the test material, Varisoft 475 (75%), did not induce repeatable increases in UDS. Treatments from 5.0 µg/ml to 0.25 µg/ml covered a

range of toxicity (68.8% to 96.4% survival) and were selected for analysis of nuclear labeling. The test material was insoluble in media at concentrations above 15 µg/ml. A borderline increase in the percentage of cells in UDS was observed in one trial, but the increase was not reproduced in a second trial. Varisoft 475 (75%) was therefore considered inactive in the Rat Primary hepatocyte UDS Assay.

Cytotoxic concentration: > 5 ug/ml

Genotoxic effects: Inactive in the Rat Primary Hepatocyte UDS Assay

Statistical results: The test material did not induce consistent changes in the nuclear labeling of rat primary hepatocytes in two independent trials for an applied concentration range of 5.00 µg/ml to 0.250 µg/ml.

Remarks:

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1A

Remarks: Reliable without restriction; guideline study.

References

Cifone, Maria A. 1989. Mutagenicity Test on Varisoft 475 (75%) in the Rat Primary Hepatocyte Unscheduled DNA Synthesis Assay. Study number 10554-1-447. Sherex Chemical Company, Inc. Dublin, OH, U. S.

Other

Last changed: July 3, 2001

Order number for sorting: 163

Remarks:

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Test Substance

Identity:	Varisoft 475 (75%) (CAS RN 68122-86-1; Imidazolium compounds, 4,5-dihydro-1-methyl-2-nortallow alkyl-1-(2-tallow amidoethyl) Me sulfate)
Purity:	76.6% in isopropyl alcohol
Remarks:	

Method

Method/guideline followed:	Not applicable (Probe study)
GLP:	Yes
Year:	1993
Species:	Rat
Strain:	Sprague-Dawley
Route of administration:	Gavage
Doses/concentration levels:	0, 200, 350, 610 and 1875 mg/kg/day
Sex:	Female
Exposure period:	Days 6 - 15 of gestation
Frequency of treatment:	
Control group and treatment:	Yes (concurrent, dosed with Milli-Q water at a dose volume equivalent to that used in the high-dose group)
Duration of test:	Days 0 - 21 of gestation
Statistical methods:	The unit of comparison was the pregnant dam or the litter. ANOVA, t-tests, Kruskal-Wallis Test, Mann-Whitney U Test and Fisher's Exact Test were used where appropriate.
Remarks:	The objective of this study was to obtain information from which to select dosage levels for a subsequent definitive rat developmental toxicity study. Timed-pregnant rats were administered the test substance by gavage on gestation days (gd) 6 through 15. Five copulation plug-positive females per group were dosed with undiluted test substance at dose levels of 200, 340, 610, 1075 and 1875 mg active ingredient/kg/day. Clinical observations were made daily (twice daily during dosing), and maternal body weights were measured on gd 0, 6, 9, 12, 15, 18 and 21. At scheduled sacrifice on gd 21, the dams were evaluated for liver and gravid uterine weights, number of corpora lutea and number and status of implantation sites (including early and late resorptions, dead fetuses and live fetuses). All live and dead fetuses were dissected from the uterus, weighed and examined for sex determinations and external malformations (including cleft palate) and variations. Fetuses were then euthanized by decapitation and discarded.

Results

Maternal toxicity NOEL:	> 1875 mg/kg/day
Developmental toxicity NOEL:	Not appropriate (probe study)
Actual dose received:	As dosed
Maternal data:	There were no treatment-related effects on clinical signs of toxicity, food consumption, gestational body weight and body weight gain, corrected body weight, corrected body weight gain, and gravid uterine weight. No treatment-related differences in gestational parameters including total number of implantations or number of viable and nonviable implants were observed in any dose group. No females died prior to scheduled sacrifice. No females aborted, delivered early or were removed from the study. At scheduled sacrifice, one female in the 1075 mg/kg/day group was found to be nonpregnant and another from this group contained only non-viable fetuses. All other females were pregnant and bore at least one viable fetus.
Fetal data:	Fetal body weights per litter were not affected by treatment. No treatment-related external malformations or variations were observed in this study.
Statistical results:	See above
Remarks:	

Conclusions

Remarks:	Administration of the test substance during organogenesis resulted in no maternal toxicity, embryotoxicity, or developmental toxicity (author of the report). The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Taskd Group).

Data Quality

Reliability (Klimisch):	1D
Remarks:	Reliable without restriction; probe study with no appropriate guideline

References

Chun, J. S. and T. L. Neeper-Bradley. 1993. Developmental Toxicity Dose Range-Finding Study of Varisoft 475 (75%) Administered by Gavage to CD® (Sprague-Dawley) Rats. EPA Document number 86-930000148. Bushy Run Research Center, Export, PA, U. S.

Other

Last changed:	July 3, 2001
Order number for sorting:	166d
Remarks:	

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Test Substance

Identity:	Varisoft 475 (75%) (CAS RN 68122-86-1; Imidazolium compounds, 4,5-dihydro-1-methyl-2-nortallow alkyl-1-(2-tallow amidoethyl) Me sulfate)
Purity:	76.6% in isopropyl alcohol
Remarks:	

Method

Method/guideline followed:	FIFRA 83-3
GLP:	Yes
Year:	1992
Species:	Rat
Strain:	Sprague-Dawley
Route of administration:	Gavage
Doses/concentration levels:	0, 100, 300 and 1000 mg/kg/day
Sex:	Female
Exposure period:	Days 6 - 15 of gestation
Frequency of treatment:	Daily
Control group and treatment:	Yes (concurrent, dosed with Milli-Q water at a dose volume equivalent to that used in the high-dose group)
Duration of test:	Days 0 - 21 of gestation
Statistical methods:	The unit of comparison was the pregnant dam or the litter. ANOVA, t-tests, Kruskal-Wallis Test, Mann-Whitney U Test and Fisher's Exact Test were used where appropriate.
Remarks:	The objective of this study was to evaluate the potential of the test substance to produce developmental toxicity when administered by a gavage to pregnant CD® rats during organogenesis. Maternal toxicity was also evaluated. Timed-pregnant rats were administered the test substance by gavage on gestation days (gd) 6 through 15. Twenty-five copulation plug-positive females per group were dosed with undiluted test substance at dose levels corresponding to 100, 300 and 1000 mg active ingredient/kg/day. An additional 25 females, assigned to the control group, received Milli-Q water at a dose volume equivalent to that used in the high dose group. Clinical observations were made daily (twice daily during dosing), and maternal body weights were measured on gd 0, 6, 9, 12, 15, 18 and 21. At scheduled sacrifice on gd 21, the dams were evaluated for liver and gravid uterine weights, number of corpora lutea and number and status of implantation sites (including early and late resorptions, dead fetuses and live fetuses). Approximately one-half of the live fetuses in each litter

were examined for visceral and craniofacial malformations and variations. The remaining one-half of the fetuses were stained with alizarin red S and were examined for skeletal malformations and variations.

Results

Maternal toxicity NOEL: > 1000 mg/kg/day

Developmental toxicity NOEL: > 1000 mg/kg/day

Actual dose received: Not stated

Maternal data: The pregnancy rate was equivalent across groups and ranged from 88 - 100%. No females aborted or delivered early. At scheduled sacrifice, three females in the control group, two females in the 100 mg/kg/day group and one female in the 300 mg/kg/day group were found to be nonpregnant. One female from the control group and one female from the 300 mg/kg/day group contained no viable fetuses at scheduled sacrifice. Twenty-one to 25 live litters were available for evaluation from each group. One female in the 300 mg/kg/day treatment group became moribund and was sacrificed on gd 10. Two to three dams in the 300 and 1000 mg/kg/day treatment groups exhibited audible respiration during or subsequent to the treatment period. None of these observations were considered to be test substance related. There were no treatment-related effects on food consumption, gestational body weight and body weight gain, corrected body weight, corrected body weight gain, and gravid uterine weight. No treatment-related differences in gestational parameters including total number of implantations, number of viable implants, and number of nonviable implants, were observed in any dose group.

Fetal data: Fetal body weights per litter were not affected by treatment. No treatment-related malformations or variations were observed in this study.

Statistical results: See above

Remarks:

Conclusions

Remarks: Administration of the test substance by gavage to pregnant rats during organogenesis resulted in no treatment-related maternal toxicity, embryotoxicity, teratogenicity, or developmental delay (author of the report).

The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1A
Remarks: Reliable without restriction; guideline study.

References

Neeper-Bradley, T. L. 1992. Developmental Toxicity Evaluation of Varisoft 475 (75%) Administered by Gavage to CD® (Sprague-Dawley) Rats. Report number 91N0034. Bushy Run Research Center, Export, PA, U. S.

Other

Last changed: July 3, 2001
Order number for sorting: 166a
Remarks:

201-15634B1

Robust Summaries
ACC FND Amides Category III - FND Amphoterics (N-carboxymethyl substituted)
September 16, 2004

Appendix 3

2.1 MELTING POINT

2.2 BOILING POINT

2.4 VAPOR PRESSURE

2.5 PARTITION COEFFICIENT

2.6 WATER SOLUBILITY

3.1.1 PHOTODEGRADATION

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

3.5 BIODEGRADATION

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

5.1.1 ACUTE ORAL TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY *IN VITRO*

5.6 GENETIC TOXICITY *IN VIVO*

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

2.1 MELTING POINT

Test Substance

Identity:	1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, hydroxide, inner salt- (CAS RN 693-33-4; 1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, inner salt)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Program (v 1.41) – The weighted mean was calculated using the values derived from the Joback Group Contribution Method and Gold and Ogle Method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Melting Point:	243 °C (weighted mean)
Decomposition:	Not applicable
Sublimation:	Not applicable
Remarks:	Following are the results from the model output (melting point only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(O)CN(CCCCCCCCCCCCCCCC)(C)C
CHEM   : 1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-,
hydroxide, inner salt-
MOL FOR: C20 H42 N1 O2
MOL WT : 328.56
--------------------- SUMMARY MPBPWIN v1.41 --------------------
Melting Point:  349.84 deg C (Adapted Joback Method)
Melting Point:  216.83 deg C (Gold and Ogle Method)
Mean Melt Pt :  283.33 deg C (Joback; Gold,Ogle Methods)
  Selected MP:  243.43 deg C (Weighted Value)

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  3  |  -CH3              |   -5.10  |  -15.30
 Group | 16  |  -CH2-             |   11.27  |  180.32
 Group |  1  |  -COOH (acid)      |  155.50  |  155.50
 Group |  1  |  >N< (+5)          |  340.00  |  340.00
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
```

RESULT	MELTING POINT in deg Kelvin	783.02
RESULT-limit	MELTING POINT in deg Kelvin	623.00
	MELTING POINT in deg C	349.84

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2

Remarks: Reliable with restrictions; model data.

References U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 7, 2004

Order Number for Sorting:

Remarks:

2.2 BOILING POINT

Test Substance

Identity:	1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, hydroxide, inner salt- (CAS RN 693-33-4; 1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, inner salt)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the adapted Stein and Brown method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Boiling Point:	566 °C
Pressure:	760 mm Hg
Decomposition:	Not applicable
Remarks:	Following are the results from the model (boiling point only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(O)CN(CCCCCCCCCCCCCCC)(C)C
CHEM   : 1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-,
hydroxide, inner salt-
MOL FOR: C20 H42 N1 O2
MOL WT : 328.56
---------------------- SUMMARY MPBPWIN v1.41 --------------------
Boiling Point:  566.00 deg C (Adapted Stein and Brown Method)
-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  3  |  -CH3              |   21.98  |   65.94
 Group | 16  |  -CH2-             |   24.22  |  387.52
 Group |  1  |  -COOH (acid)      |  169.83  |  169.83
 Group |  1  |  >N< (+5)          |  340.00  |  340.00
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  | 1161.47
RESULT- corr |  BOILING POINT in deg Kelvin  |  839.16
             |  BOILING POINT in deg C       |  566.00
-----------------------------------------------------
```

Conclusions

The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 7, 2004
Order Number for Sorting:
Remarks:

2.4 VAPOR PRESSURE

Test Substance

Identity:	1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, hydroxide, inner salt- (CAS RN 693-33-4; 1-Hexadecanaminium, N-carboxymethyl)-N,N-dimethyl-, inner salt)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) MPBPWIN Submodel (v 1.41) – Estimated value was obtained using the Modified Grain method.
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 109 °C and boiling point of 250 °C.

Results

Vapor Pressure:	2.4 E-12 mmHg
Temperature:	25°C
Decomposition:	Not applicable
Remarks:	Following are the results from the model (vapor pressure only):

```
MPBPWIN (v1.41) Program Results:
================================
Experimental Database Structure Match:  no data

SMILES : O=C(O)CN(CCCCCCCCCCCCCCCC)(C)C
CHEM   : 1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-,
hydroxide, inner salt-
MOL FOR: C20 H42 N1 O2
MOL WT : 328.56
--------------------- SUMMARY MPBPWIN v1.41 --------------------

Vapor Pressure Estimations (25 deg C):
  (Using BP: 566.00 deg C (estimated))
  (Using MP: 243.43 deg C (estimated))
    VP:  2.22E-015 mm Hg (Antoine Method)
    VP:  2.42E-012 mm Hg (Modified Grain Method)
    VP:  8.28E-012 mm Hg (Mackay Method)
  Selected VP:  2.42E-012 mm Hg (Modified Grain Method)
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; MPBPWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 7, 2004
Order Number for Sorting:
Remarks:

2.5 PARTITION COEFFICIENT

Test Substance

Identity:	1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, hydroxide, inner salt- (CAS RN 693-33-4; 1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, inner salt)
Purity:	Not applicable

Method

Method:	EPIWIN (v 3.11), KOWWIN Program (v 1.67)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run with the following physico-chemical property input values: melting point of 109 °C and boiling point of 250 °C.

Results

Log K_{ow}:	2.44
Temperature °C:	Not stated
Remarks:	Following are the results from the model:

```
KOWWIN Program (v1.67) Results:
===============================

                  Log Kow(version 1.67 estimate): 2.44

SMILES : O=C(O)CN(CCCCCCCCCCCCCCCC)(C)C
CHEM   : 1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, hydroxide, inner
          salt-
MOL FOR: C20 H42 N1 O2
MOL WT : 328.56
-------+-----+---------------------------------------+---------+--------
 TYPE  | NUM |        LOGKOW FRAGMENT DESCRIPTION    |  COEFF  | VALUE
-------+-----+---------------------------------------+---------+--------
 Frag  |  3  |  -CH3    [aliphatic carbon]           | 0.5473  |  1.6419
 Frag  | 16  |  -CH2-   [aliphatic carbon]           | 0.4911  |  7.8576
 Frag  |  1  |  -COOH   [acid, aliphatic attach]     |-0.6895  | -0.6895
 Frag  |  1  |  >N<     [+5 valence; single bonds;   |-6.6000  | -6.6000
       |     |           no H attach]                |         |
 Const |     |  Equation Constant                    |         |  0.2290
-------+-----+---------------------------------------+---------+--------
                                                 Log Kow   =   2.4390
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability:	2
Remarks:	Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; KOWWIN Program, Version 1.67; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed:	July 7, 2004
Order Number for Sorting:	
Remarks:	

2.6 WATER SOLUBILITY

Test Substance

Identity:	1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, hydroxide, inner salt- (CAS RN 693-33-4; 1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, inner salt)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11), WSKOWWIN Program (v 1.41)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Solubility:	171 mg/L
Temperature:	25°C
pH value and concentration:	Not stated
pKa value at 25°C:	Not stated
Remarks:	Following are the results from the model:

```
Water Sol from Kow (WSKOW v1.41) Results:
=========================================

          Water Sol: 170.9 mg/L

SMILES : O=C(O)CN(CCCCCCCCCCCCCCC)(C)C
CHEM   : 1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, hydroxide,
inner
          salt-
MOL FOR: C20 H42 N1 O2
MOL WT : 328.56
---------------------- WSKOW v1.41 Results --------------------
Log Kow  (estimated)  :  2.44
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  2.44

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      --------------------   -----
       Acid, aliphatic       0.395

   Log Water Solubility  (in moles/L) :  -3.284
Water Solubility at 25 deg C (mg/L):  170.9
```

Conclusions The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; WSKOWWIN Program, Version 1.41; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last Changed: July 7, 2004
Order Number for Sorting:
Remarks:

3.1.1 PHOTODEGRADATION

Test Substance

Identity:	1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, hydroxide, inner salt- (CAS RN 693-33-4; 1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, inner salt)
Purity:	Not applicable

Method

Method/guideline followed:	EPIWIN (v 3.11), AOPWIN Program (v 1.91)
Type:	Not applicable
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Concentration of substance:	Not applicable
Temperature (°C):	Not stated
Direct photolysis:	Not stated
Indirect photolysis:	Not stated
Breakdown products:	Not applicable
Remarks:	Overall OH Rate Constant: (k_{phot}) = 40 cm^3/molecule-sec; Half life: $t_{1/2}$ = 3.2 hrs

Following are the results from the model:

```
AOP Program (v1.91) Results:
============================
SMILES : O=C(O)CN(CCCCCCCCCCCCCCCC)(C)C
CHEM   : 1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, hydroxide,
         inner salt-
MOL FOR: C20 H42 N1 O2
MOL WT : 328.56
---------------- SUMMARY (AOP v1.91): HYDROXYL RADICALS -----------------
Hydrogen Abstraction         =  39.4140 E-12 cm3/molecule-sec
**Reaction with N, S and -OH =   0.5200 E-12 cm3/molecule-sec
Addition to Triple Bonds     =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings   =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings      =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  39.9340 E-12 cm3/molecule-sec
   HALF-LIFE =     0.268 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =     3.214 Hrs
** Designates Estimation(s) Using ASSUMED Value(s)
```

```
--------------- SUMMARY (AOP v1.91): OZONE REACTION --------------------

               ******  NO OZONE REACTION ESTIMATION ******
               (ONLY Olefins and Acetylenes are Estimated)

Experimental Database:  NO Structure Matches
```

Conclusions	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions; model data

References	U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; AOPWIN Program, Version 1.91; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other

Last changed:	July 7, 2004
Order number for sorting:	
Remarks:	

3.3.2 TRANSPORTATION BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY MODEL)

Test Substance

Identity:	1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, hydroxide, inner salt- (CAS RN 693-33-4; 1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-, inner salt)
Purity:	Not applicable

Method

Method/Guideline followed:	EPIWIN (v 3.11) Level III Fugacity Model; adapted from Mackay's EQC Level III Fugacity Model Media: Water, air, soil and sediment (model run with 1000 kg/hr emissions to water and 0 kg/hr emissions to air, soil and sediment)
GLP:	Not applicable
Year:	2004
Remarks:	The EPIWIN model was run without entering measured physical chemical properties.

Results

Remarks:	Following are the results from the model:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : 1-Hexadecanaminium, N-(carboxymethyl)-N,N-dimethyl-,
                hydroxide, inner salt-
  Molecular Wt: 328.56
  Henry's LC  : 4.34e-014 atm-m3/mole (Henrywin program)
  Vapor Press : 2.42e-012 mm Hg  (Mpbpwin program)
  Liquid VP   : 3.5e-010 mm Hg  (super-cooled)
  Melting Pt  : 243 deg C (Mpbpwin program)
  Log Kow     : 2.44  (Kowwin program)
  Soil Koc    : 113  (calc by model)

            Mass Amount    Half-Life    Emissions
             (percent)        (hr)       (kg/hr)
   Air       2.01e-012       6.43         0
   Water     99.5            360          1000
   Soil      1.97e-008       360          0
   Sediment  0.489           1.44e+003    0

              Fugacity    Reaction    Advection   Reaction    Advection
               (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       1.99e-027    7.42e-010   6.88e-011    7.42e-011   6.88e-012
   Water     2.26e-019    658         342          65.8        34.2
   Soil      1.65e-028    1.3e-007    0            1.3e-008    0
   Sediment  1.49e-019    0.808       0.0336       0.0808      0.00336
```

```
Persistence Time: 343 hr
Reaction Time:    521 hr
Advection Time:   1e+003 hr
Percent Reacted:  65.8
Percent Advected: 34.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      6.427
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 3.136  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Conclusions:

Mass Amounts:
Air < 1 %
Water = 99 %
Soil < 1%
Sediment = 0.5 %

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability: 2
Remarks: Reliable with restrictions; model data.

References

U.S. EPA (U.S. Environmental Protection Agency). 2000. EPI Suite, Version 3.11; Level III Fugacity Model; PC-Computer software developed by EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).

Other Available Reports

Other

Last changed: July 7, 2004
Order number for sorting:
Remarks:

3.5 BIODEGRADATION

Test Substance

Identity:	Betadet HR (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivatives, inner salt)
Purity:	31% active ingredient, 35% dry matter
Remarks:	

Method

Method/Guideline followed:	OECD Guideline for Testing of Chemicals (1981) No. 301D referenced as Method C.6 of Commission Directive 84/449/EEC
Test type:	Closed bottle
GLP:	Yes
Year:	1991
Contact time:	28 days
Inoculum:	Activated sludge bacteria from the aeration stage of the Severn Trent Plc sewage treatment plant at Belper, Derbyshire
Remarks:	The test assessed the ready biodegradability of the test substance in the Closed Bottle Test. 250 - 300 ml BOD bottles (darkened glass) with ground glass stoppers were filled with standard culture medium and the following test concentrations: a. Non-inoculated culture medium; b. 1 drop/l inoculum; c. 2 mg ai/l test material and 1 drop/l inoculum; and d. 3 mg/l sodium benzoate and 1 drop/l inoculum. The bottles were stoppered firmly. Sufficient bottles were prepared to allow a single oxygen determination per bottle to be made at 0, 5, 15 and 28 days for each test medium (duplicate bottles at each sampling time). Dissolved oxygen concentrations were measured by means of a Yellow Springs BOD Probe (Model 54). Chemical Oxygen Demand was determined using a semi-micro sample digestion (Hach) technique. Reaction vials containing premeasured amounts of sulphuric acid, potassium dichromate, silver catalyst plus 2 ml water sample were heated at 150 °C for 2 hours and the COD values read from a Hach DR/2000 Direct Reading Spectrophotometer.

Results

Degradation:

Mean Oxygen Depletion and Percentage Biodegradation Values				
Test Series		Day 5	Day 15	Day 28
Culture medium, no inoculum	O_2 depletion (mg O_2/l)	0.100	0.175	0.200
	% degradation			
Culture medium plus inoculum	O_2 depletion (mg O_2/l)	0.125	0.275	0.300
	% degradation			
2 mg ai/l test material plus inoculum	O_2 depletion (mg O_2/l)	1.525	2.850	3.250
	% degradation (% of COD)	44	82	93
3 mg/l sodium benzoate plus inoculum	O_2 depletion (mg O_2/l)	3.600	4.600	4.675
	% degradation (% of ThOD)	72	92	93
	% degradation (% of COD)	73	93	95

Results: Sodium benzoate attained 95% degradation within 28 days. Oxygen depletions in the inoculated and non-inoculated control series were within the prescribed limits:
Non-inoculated control: < 0.3 mg O_2/l after 5 days
< 0.4 mg O_2/l after 28 days
Inoculated control: < 0.5 mg O_2/l after 5 days
< 0.6 mg O_2/l after 28 days

Kinetic: None stated
Breakdown products: None stated
Remarks:

Conclusions

Remarks: Betadet HR attained 93% degradation (% of COD) within 28 days and therefore, can be considered readily biodegradable under the strict terms and conditions of OECD Guideline No. 301 D (author of the report).
The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Handley, J. W. and I. G. Sewell. 1991. Assessment of Ready Biodegradability (Closed Bottle Test) of Betadet HR. Project number 309/35. SafePharm Laboratories, Derby, U. K. Sponsored by Kao Corporation S.A.

Other Available Reports

Other

Last changed:	October 29, 2001
Order number for sorting:	157b
Remarks:	

3.5 BIODEGRADATION

Test Substance

Identity:	Dehyton K (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivatives, inner salt)
Purity:	29 - 32% active ingredient (AI) in water
Remarks:	Impurities: ca. 5% NaCl; ≤ 0.3% Amidoamine

Method

Method/Guideline followed:	OECD Guideline 301D (Ready Biodegradability: Closed Bottle Test)
Test type:	Aerobic ready biodegradability
GLP:	Yes
Year:	1996
Contact time:	28 days
Inoculum:	Sewage treatment plant effluent (predominantly domestic)
Remarks:	The test substance was measured for ready biodegradability in a closed bottle system. Aliquots of stock solution at concentrations of 2 and 5 mg/l were transferred to a mineral nutrient solution, inoculated with purification plant effluent and poured, without air bubbles, into bottles of known volume. The closed bottles were incubated at a constant 20 ± 1 °C in the dark or in diffused light and the biochemical oxygen demand of the test substance was measured using the Winkler Titration Method. Biodegradability was calculated as %BOD/ThOD or %BOD/COD. As a reference substance, an inoculated nutrient solution containing inoculant consumption control (IZK) and sodium benzoate was tested as well.

Results

Degradation: 86% degradation in 28 days

Results:

Biodegradability in the Closed Bottle Test					
Test substance	**Test concentration (mg/l)**	**In relation to**	**% BOD/COD or ThOD after x Days**		
			7	**21**	**28**
Sodium benzoate	2	substance	75	93	96
Dehyton K	2	AI	40	80	86
	5	AI	54	75*	75*

* Insufficient residual oxygen in test system.

Kinetic: See table

Breakdown products:	None stated
Remarks:	A trial was deemed as valid when the degradation values of the replicates of the test substance did not deviate more than 20% at the end of the test or at the end of the 14-day window, and when the percent degradation of the reference substance reached the plateau for ready biodegradability (60% BOD/ThOD or BOD/COD) within 14 days. Test substances can be graded as readily biodegradable when the plateau for ready biodegradability is reached within 14 days after that time period when the biodegradability exceeds 10% for the first time (14-day window). The total test time for this may not exceed 28 days.

Conclusions

Remarks:	The test substance was considered readily biodegradable. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Werner and Berger. 1996. Dehyton K: Closed Bottle/EG-RILI. Final Report. Report number R 9501454. Henkel KGaA, Research Biology/Product Safety Ecology, Düsseldorf, Germany.

Other Available Reports

Other

Last changed:	October 29, 2001
Order number for sorting:	157s
Remarks:	

3.5 BIODEGRADATION

Test Substance

Identity:	1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivs., inner salt (CAS RN 61789-40-0)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Methods conformed to OECD Guideline 301B
Test type:	Aerobic ready biodegradability
GLP:	Not stated
Year:	1994
Contact time:	35 days
Inoculum:	Activated sludge
Remarks:	Three liters of mineral nutrient solution were added to each of five, 5-l carboys. To two carboys were added test substance (equivalent concentrations to achieve 10 and 20 mg organic carbon/l), two carboys were maintained as blank test flasks, and one carboy was added reference substance (aniline) at 20 mg organic carbon/l. Inoculum was added to all carboys (30 ml containing 10^8 cells/ml), and the carboys were aerated with CO_2-free air (30 – 50 ml/minute) with the effluent air passing through a series of CO_2 traps containing $Ba(OH)_2$. The CO_2 produced by the degradation of the test substance by the inoculum was subsequently trapped in the $Ba(OH)_2$ solution. The amount of CO_2 produced was determined by titrating the $Ba(OH)_2$ with HCl. Biodegradation was determined in two manners. First, biodegradation was calculated as the amount of CO_2 collected in the trapping solution divided by the amount of CO_2 that could theoretically have been produced based on the amount of carbon (as test substance) added to the test vessels. Second, biodegradation was measured as the amount of dissolved organic carbon removed from the test vessels. The target temperature for the test was 21 ± 1 °C.

Results

Degradation:	Evidence of ready biodegradability was demonstrated in this test; pass levels for this test were 60% evolution of the theoretical CO_2 and 70% removal of the dissolved organic carbon
Results:	Evolution of CO_2 in the 10 mg organic carbon/l treatment was 71 and 71% at days 29 and 35, respectively. Evolution

of CO_2 in the 20 mg organic carbon/l treatment was 57 and 58% at days 29 and 35, respectively. Percent removal of dissolved organic carbon in the 10 mg organic carbon/l treatment was 88.5 and 93% at 29 days and 35 days, respectively. Percent removal of dissolved organic carbon in the 20 mg organic carbon/l treatment was 81 and 90%, respectively.

Kinetic: % Degradation

Day	Test Substance 10 mg/L	Test Substance 20 mg/L	Reference Substance
4	11	14	16
13	59	48	72
29	71	57	83
35	71	58	82

Breakdown products: Not stated
Remarks:

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2C
Remarks: Reliable with restrictions; comparable to guideline study with acceptable restrictions.

References

Bazzon, M. and E. Thybaud. 1994. Test Report: Ready Biodegradability, CO_2 Evolution Test (Modified Sturm Test), Evaluation, in an Aqueous Medium, of the Biodegradability of Substances: 1736-15A, 1736-15B, 1736-15C, 1736-15D, 1736-15E. Report number 16BA51. Institut National de L'Environnement Industriel et des Risques, Verneuil-en-Halatte, France.

Other Available Reports

Other

Last changed: July 24, 2000
Order number for sorting: 83
Remarks:

3.5 BIODEGRADATION

Test Substance

Identity: Dehyton K; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derives., hydroxides, inner salt (CAS RN 61789-40-0)

Purity: Not stated

Remarks:

Method

Method/Guideline followed: EEC-Directive 92/69/EEC Annex V, Part C: Methods for the Determination of Ecotoxicity. C.4. Biodegradation: Determination of the Ready Biodegradability C.4-B. This test corresponds to OECD test method 301 E.

Test type: Aerobic ready biodegradation: Modified OECD Screening Test

GLP: No

Year: 1984

Contact time: 28 days

Inoculum: Effluent from a municipal sewage treatment plant

Remarks: Flasks containing mineral medium and a known concentration of the test substance (10 mg DOC/l) as the sole source of organic carbon, were shaken and inoculated with effluent of a municipal sewage treatment plant (0.5 ml/l). They were shaken again in the dark or diffuse light at 22 ± 2 °C. Degradation was followed by DOC analysis of test samples at frequent intervals during the 28-day period. The degree of biodegradation was calculated by expressing the concentration of DOC removed (corrected for DOC in the blank inoculum control) as a percentage of the concentration initially present.

Results

Degradation:

Test Concentration	**% DOC Removal After x Days**			
	7	**14**	**21**	**28**
5 mg C/l	58	98	92	100
10 mg C/l	58	90	85	100

Results: Based on the data received Dehyton K met the OECD criteria for ready biodegradability (> 70% DOC removal within a 10 day time window).

Kinetic: Not stated

Breakdown products: Not stated

Conclusions

Remarks:	The test substance is readily biodegradable. The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; data are reliable but article lacks details.

References

Steber, J. and K. Richterich. 2000. Aerobic Biodegradation: Modified OECD Screening Test. , Report No. R 0001215. Henkel KGaA, Germany.

Other Available Reports

Other

Last changed:	October 29, 2001
Order number for sorting:	157n
Remarks:	

3.5 BIODEGRADATION

Test Substance

Identity: Dehyton K, 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derives., hydroxides, inner salt
(CAS RN 61789-40-0)

Purity: Not stated

Remarks:

Method

Method/Guideline followed: 87/302/EEC Commission Directive of 18. November 1987 (part C: Zahn-Wellens-Test). This test corresponds to OECD test method 302 B.

Test type: Aerobic biodegradation

GLP: No

Year: 1984

Contact time: 28 days

Inoculum: Activated sludge

Remarks: Activated sludge, mineral nutrients and test substance in aqueous medium at 50 – 400 mg dissolved organic carbon (DOC)/l were contained in a 1 – 5 liter glass vessel, equipped with a magnetic stirrer and an aerator. The mixture was stirred and aerated at 20 –25 °C in the dark or in diffuse light for up to 28 days. Blank controls, containing activated sludge and mineral nutrients but no test substance, are run in parallel. The biodegradation process was monitored by determination of DOC values in filtered samples taken at daily or other time intervals. The ratio of eliminated DOC, corrected for the blank, after each time interval to the initial DOC value was expressed as the percentage biodegradation at the sampling time.

Results

Degradation:

Test Concentration	**% DOC Removal After x Days**			
	7	**14**	**21**	**28**
250 mg/l	65	71	71	100
500 mg/l	70	100	99	97

Results: Based on these data, Dehyton K can be regarded as inherently biodegradable.

Kinetic: See table above

Breakdown products:	None stated
Remarks:	

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; data are reliable but article lacks details.

References

Steber, J. and K. Richterich. 2000. Aerobic Biodegradation: Zahn-Wellens-Test. Unpublished Results; Test Substance Registration number 6492, Test Run number 12. Report No. R 0001216. Henkel KGaA, Biological Research and Product Safety/Ecology, Germany.

Other Available Reports

Other

Last changed:	July 3, 2001
Order number for sorting:	157o
Remarks:	

3.5 BIODEGRADATION

Test Substance

Identity:	1-Propanaminium, 3-amino-N- (carboxymethyl)-N,N-dimethyl-, N-coco acyl derivs., hydroxides, inner salt (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivs., inner salt)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	OECD Guideline 303A, Coupled Units Test (Model Sewage Treatment Plant)
Test type:	Aerobic ready biodegradability
GLP:	Not stated
Year:	1999
Contact time:	Not stated
Inoculum:	Activated sludge
Remarks:	Two OECD Confirmatory Test units (i.e. model activated sludge plants were run in parallel. Test material (10 – 20 mg DOC/l) was added to the influent (synthetic sewage) of one unit while the second unit was fed only synthetic sewage. The DOC concentrations were measured in both effluents. The DOC difference of the effluent values was due to non- or partially degraded test material.

Results

Degradation:	At a test concentration of 10 mg C/l, and a hydraulic retention time of 3 hours, the carbon elimination (DOC removal) was 97 ± 4%
Results:	Based on the data, the test substance was regarded as biodegradable and accessible to elimination under the conditions of the test.
Kinetic:	Not stated
Breakdown products:	Not stated
Remarks:	

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Reliable with restrictions: data are reliable but article lacks details, comparable to guidelines/standards.

References

Steber, J. and H. Berger. 1999. Biological Research and Product Safety/Ecology. Report number 1988/2648. Henkel KGaA, Duesseldorf, Germany.

Steber, J. and H. Berger. 1999. Biological Research and Product Safety/Ecology: unpublished results. Test substance registration number Fi 7208. Henkel KGaA, Duesseldorf, Germany.

Other Available Reports

Other

Last changed:	August 1, 2000
Order number for sorting:	82
Remarks:	

3.5 BIODEGRADATION

Test Substance

Identity:	Dehyton Ke 3133 (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivatives, inner salt)
Purity:	29 – 32% active ingredient in water
Remarks:	

Method

Method/Guideline followed:	Guideline for screening of chemicals for anaerobic biodegradability (Annex 1) of the ECETOC-Technical Report number 28
Test type:	Anaerobic biodegradability
GLP:	Yes
Year:	1995
Contact time:	56 days
Inoculum:	Anaerobic organisms of the purification plant Hilden
Remarks:	The calculation of the anaerobic biodegradability of Dehyton Ke 3133 was carried out in the ECETOC-Screening test inoculated with anaerobic organisms of the Hilden purification plant. The digester sludge was coarsely sifted and 1.5 liters of sludge were washed and diluted with a mineral nutrient medium to 20 liters total volume. The dry weight determination of the inoculated nutrient medium revealed a dry weight content of 0.39%. Test and control concentrations were tested in 5 parallels. At the beginning of the test, the pH of the test suspension was 7.05. The end pH value in all test assays was 6.7 – 6.9. Incubation temperature was 35 ± 2 °C. Test concentrations were 50 or 100 mg AS/l. Gas pressure measurements were taken at the beginning and end , as well as once per week. At the end of the trial, the dissolved inorganic carbon was determined in an aliquot of suspension supernatant using a C-analyzer. In the course of the 56-day anaerobic incubation of the test substance (test concentration 50 or 100 mg AS/l) at 35 °C, the digester gas was tracked by pressure measurements and at the end of the trial the total biodegradability was calculated from the digester gas and dissolved inorganic carbon measurements.

Results

Degradation:

Biodegradation (% of Organic Carbon in the Test Substance)				
Test Substance	**Concentration**	**Gas Development**	**DIC Production**	**Total Biodegradation**
Dehyton Ke 3133	50 mg/l	38.0	59.6	97.6 ± 18.6
	100 mg/l	32.7	23.6	56.3 ± 17.0

Results: The test substance was considered biodegradable.
Kinetic: None stated
Breakdown products: None stated
Remarks: While pressure measurements independent of the test concentrations produced comparable results (38.0% or 32.7% of the theoretical digester gas development), the DIC measurements at the end of the test produced considerable differences (59.6% or 23.6% of the theoretical digester gas development). The calculated total biodegradation was, therefore, considerably higher for the 50 mg/l test concentration than for the 100 mg/l concentration. Comparison of the theoretical CH_4/CO_2 ratio using the Buswell equation (approx. 70% CH_4/30% CO_2) with the CO_2 experimental value for the 50 mg/l test substance, indicated the experimental value was too high. Therefore, the results for the 100 mg/l test sample were used.

Conclusions

Remarks: Dehyton Ke 3133 is at least partially anaerobically biodegradable (author of report). The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1A
Remarks: Reliable without restriction; guideline study.

References

Richterich, K. 1995. Dehyton Ke 3133: Anaerobic Biodegradability in the ECETOC Test. Report number R 9500675. Henkel KGaA, Research Biology Ecology, Düsseldorf, Germany.

Other Available Reports

Other

Last changed:	October 29, 2001
Order number for sorting:	157t

3.5 BIODEGRADATION

Test Substance

Identity:	ANFODAC LB – alchil (C12) ammido propil betaina (CAS RN 4292-10-8; 1-Propanaminium, N-(carboxymethyl)-N,N-dimethyl-3-[(1-oxododecyl)amino]-, inner salt)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	MITI test modified, according to the provisions of CEE Directive 92/69.
Test type:	Aerobic
GLP:	Not stated
Year:	1996
Contact time:	28 days
Inoculum:	From a purifying plant for home and industrial effluents, from an industrial effluent purifying plant and surface water and river surface soil.
Remarks:	A one liter sample each was drawn from the mud recycling line in a liquid urban effluent treatment plant, mud recycling line in a liquid industrial effluent treatment plant, surface water from a river, and surface soil from the bank of a river. The samples of the drawn muds were mixed in a single container and the mixture was left to rest. The foreign and floating substances were taken away and the supernatant was filtered through filter paper. The filtered substance was aerated. The test material was used at a concentration of 100 mg/l. All samples were tested in duplicate. The reference substance was sodium benzoate. The percent degradation on the basis of the oxygen consumption was evaluated. Percentage degradation = [(BOD - B)/COD] x 100, where BOD = biological oxygen demand; B = oxygen consumption of the culture soil added to the inoculation; and COD = chemical oxygen demand . The oxygen biochemical requirement was measured with a respirometer. The test is considered valid when the degradation percentage of the sodium benzoate exceeds 40% after 7 days and 65% after 14 days. The test substance is considered readily biodegradable when the degradation percentage obtained is equal to or higher than 60%.

Results

Degradation:	The percent biodegradability was 82% after 28 days, using the ThOD value (0.70 mg O_2/mg). The percentage of biodegradability was 95% after 28 days, using the COD value (60 mg/l).
Results:	Based on the degradation rate, the test substance was readily biodegradable.
Kinetic:	Not stated
Breakdown products:	Not stated
Remarks:	

Conclusions

Remarks:	The test substance was readily biodegradable. The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1C
Remarks:	Reliable without restriction: test procedure according to national standards.

References

Biffi, E. 1996. Biodegradability Tests: Test Material: ANFODAC LB. Unpublished Report (Project number 96/200.A6). Biolab, Italy.

Other Available Reports

Other

Last changed:	July 3, 2001
Order number for sorting:	168
Remarks:	

3.5 BIODEGRADATION

Test Substance

Identity:	Hoe S 3267 (CAS RN 70851-07-9; Amides, coco, N-[3-(dimethylamino)propyl], alkylation products with chloroacetic acid, sodium salts)
Purity:	Approximately 30%
Remarks:	

Method

Method/Guideline followed:	Modified Zahn-Wellens; DIN 38 412 Part 25, 88/302/EWG (Part C), 302 B in the OECD Guidelines, and DIN 38 409 Part 3.
Test type:	Aerobic biodegradability
GLP:	Not stated
Year:	1986
Contact time:	34 days
Inoculum:	Centrifuged wet sludge
Remarks:	The test substance was measured for biodegradability in a closed bottle system. DOC determination (dissolved organic carbon content) of the stock solution was 2316 mg/l; COD of the stock solution was 4229 mg/l (O_2); DOC per 1 gram of test material was 232 mg/g (in the original solution); and COD per 1 gram of test material was 423 mg/g (O_2) (in the original solution). 12 g/l of centrifuged wet sludge were used as inoculum, corresponding to approximately 1000 mg/l dry weight. 86.5 ml/l of stock solution was used in the test assay, corresponding to 200 mg/l dissolved organic carbon content. Incubation temperature was 21 ± 1 °C. The composition of the reaction medium followed the requirements of the cited DIN Guideline. The activity of the inoculum was checked by the use of a reference assay, and a control without test substance was used. Test vessels were 2-liter beakers covered with large watchglasses. Air was blown in over large Pasteur pipettes, and the sludge was kept in suspension with a magnetic stirrer.

Results

Degradation:	> 70% in 11 days > 90% in 13 days
Results:	The test substance was inherently biodegradable.

Kinetic: % Degradation

Day	Test Substance	Reference Substance
0.13	0	2
1	< 20	0
4	20-50	30
6		63
8		97
11	>70	102
13	>90	

Breakdown products: None stated

Remarks: Seven days after adaptation, the biodegradation reached 45%. The adaptation phase (time until the beginning of significant degradation) was 1 day.

Conclusions

Remarks:	Hoe S 2367 is readily biodegradable in the Zahn-Wellens-Test (author of the report). This method is no longer used for "ready" biodegradation; the test substance was inherently biodegradable (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group). The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Voelskow, H. 1986. Report Developed from Archived Data from 1986. Study of the Biodegradability of Hoe S 2367. Hoechst AG, Germany.

Other Available Reports

Other

Last changed:	July 3, 2001
Order number for sorting:	171
Remarks:	

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	1-Propanaminium, 3 amino-N-(carboxymethyl)-N,N-dimethyl-, N-dimethyl-, N-coco acyl derivs., chlorides (CAS RN 61789-39-7; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N- dimethyl-, N-coco acyl derivs., chlorides, sodium salts)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Methods conformed to U. S. EPA TSCA, 40 CFR 797, Guideline 797.1400
Type:	Static
GLP:	Yes
Year:	1992
Species/Strain/Supplier:	Fathead minnow (*Pimephales promelas*)/laboratory culture
Analytical monitoring:	No
Exposure period:	96 hours
Statistical methods:	LC_{50} value was calculated using computer program (Stephan, C. E., K. A. Busch, R. Smith, J. Burke and R. W. 1978. A computer program for calculating an LC_{50}. U. S. Environmental Protection Agency, Duluth, MN.) using probit, moving average, or nonlinear interpolation estimates.
Remarks:	The study measured the acute toxicity of the test substance to Fathead minnows during a 96-hour exposure period. The toxicity test was conducted in 5-gallon glass vessels holding 15 liters of test solution. Dilution water was a blend of naturally hard well water and well water that had been demineralized by reverse osmosis. The blended water was prepared to contain a total hardness of 130 – 160 mg $CaCO_3$/l. Test concentrations were prepared by transferring aliquots of an aqueous stock solution of the test substance directly to 15 liters of dilution water. Concentrations were prepared on a total compound basis. Five test concentrations and a dilution water control were used in the test. Treatment groups were replicated twice, with each test vessel holding 10 fish (20 per treatment group). Fish were added to the exposure solutions within 30 minutes after preparing the exposure solutions. Test fish were reared at the test laboratory in well water and fed a diet of commercial fish food and brine shrimp. They were approximately 17 weeks old at the time of testing. A sublot

of the fish was segregated 48 hours prior to test initiation and acclimated during that time to the blended dilution water. Fish were not fed during acclimation or testing. Fish used in testing had a mean wet weight of 0.25 g and a mean standard length of 26 mm. The test chamber biomass was 0.17 g/l for the test. Test chambers were housed in a water bath at 22 ± 1 °C. A 16-hour light/8-hour dark photoperiod was maintained and light intensity over the test chambers ranged from 720 – 880 lux during the test. Measurements of temperature, dissolved oxygen and pH were made at 0, 48 and 96 hours. Temperature ranged from 22 – 23 °C, dissolved oxygen ranged from 5.7 – 8.0 mg/l in vessels with surviving fish, and pH ranged from 7.3 – 8.0. Test fish were observed every 24 hours for mortality and sublethal effects. Endpoint results were based on nominal test concentrations.

Results

Nominal concentrations (mg/l):	0 (control), 0.056, 0.10, 0.18, 0.32, and 0.56
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
Element value:	96-hour LC_{50}
Statistical results:	96-hour LC_{50} = 0.23 mg/l (95% confidence limits: 0.18 and 0.32 mg/l)
Remarks:	Additional calculated endpoints were: 24-hour LC_{50} = 0.23 mg/l (0.18 – 0.32 mg/l) 48-hour LC_{50} = 0.23 mg/l (0.18 – 0.32 mg/l) 72-hour LC_{50} = 0.23 mg/l (0.18 – 0.32 mg/l) NOEC = 0.10 mg/l Complete mortality in the 0.32 and 0.56 mg/l test levels had occurred within the first 24 hours. One fish (5%) in the 0.18 mg/l level died; all remaining fish in that level appeared normal. No mortalities occurred in any other treatment group or control.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Sword, M. C. and K. R. Thompson. 1992. Static Acute Toxicity of Miramine TO-DT to Fathead Minnow (*Pimephales promelas*). Report number 40340. ABC Laboratories, Inc., Columbia, MO, U. S.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	78
Remarks:	

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivs., hydroxides, inner salt (CAS 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivs., inner salt)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Methods conformed to EU Commission Directive 92/69/EEC. Annex. Part C: Method for the determination of ecotoxicity, C.1, method corresponds to OECD Guideline 203
Type:	Static-renewal
GLP:	Not stated
Year:	2000
Species/Strain/Supplier:	Zebra fish (*Brachydanio rerio*)
Analytical monitoring:	Not stated
Exposure period:	96 hours
Statistical methods:	Not stated
Remarks:	The experiment measured the 96-hour acute toxicity of the test substance to Zebra fish in a static-renewal test system. Test medium was renewed daily. Ten fish were exposed to each treatment level. Mortalities were recorded at least every 24 hours. The following values were calculated: LC_0 = Highest concentration showing no mortality LC_{50} = Concentration showing 50% mortality LC_{100} = Lowest concentration in which all animals died.

Results

Nominal concentrations (mg/l):	Not stated
Measured concentrations (mg/l):	Not stated
Unit:	mg of product/l
Element value:	96-hour LC_{50}
Statistical results:	96-hour LC_{50} = 6.7 mg of product/l (= 2.0 mg active matter/l)
Remarks:	Additional results calculated were: LC_0 = 5.6 mg of product/l (= 1.7 mg active matter/l) LC_{100} = 8.0 mg of product/l (= 2.4 mg active matter/l.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Reliable with restrictions; basic data given, comparable to guidelines/standards.

References

Steber, J. and H. Berger. 1999. Biological Research and Product Safety/Ecology: unpublished results; Test substance registration number Fi 6492. Henkel KGaA, Duesseldorf, Germany.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	84
Remarks:	

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	TEGO® Betain L 7 F (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivs., inner salt)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	OECD Guideline 203, bzw. Anhang zur Richtlinie 92/69 EWG Teil C.1
Type:	Static
GLP:	Not stated
Year:	1995
Species/Strain/Supplier:	Zebra fish (*Brachydanio rerio*)
Analytical monitoring:	Not stated
Exposure period:	96 hours
Statistical methods:	Not stated
Remarks:	

Results

Nominal concentrations (mg/l):	Not stated
Measured concentrations (mg/l):	Not stated
Unit:	mg/l product and mg/l active substance
Element value:	96-hour LC_{50}
Statistical results:	96-hour LC_{50} = 6.7 mg/l product = 2.0 mg/l active substance
Remarks:	Additional endpoints included: 96-hour LC_0 = 5.6 mg/l product = 1.7 mg/l active substance 96-hour LC_{100} = 8.0 mg/l product = 2.4 mg/l active substance

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Reliable with restrictions; basic data given, comparable to guidelines/standards.

References

1995. Akute Fischtoxizitaet fuer TEGO ® Betain L 7 F. Report number bet7fi. Th. Goldschmidt AG.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	86b
Remarks:	

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Betadet HR (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivatives, inner salt)
Purity:	28.5-30.5 % active ingredient
Remarks:	

Method

Method/Guideline followed:	Protocol number 203 of 4th April 1984, from the OECD Guideline for Testing of Chemicals
Type:	Static
GLP:	Yes
Year:	1992
Species/Strain/Supplier:	Zebra fish (*Brachydanio rerio*)/Not stated/Meridiana Aquarium
Analytical monitoring:	No
Exposure period:	96 hours
Statistical methods:	As the mortality data obtained in the study are inadequate for the use of standard methods of calculating the LC_{50}, the highest concentration causing no mortality and the lowest concentration producing 100 percent mortality were used as an approximation for the LC_{50} (this was considered as the geometric mean of these two concentrations).
Remarks:	The study assessed the acute toxicity of the test substance to *Brachydanio rerio* over a 96-hour period. A total of 74 male zebra fish were used in the study. They were acclimatized in a 300 liter tank for 12 days before treatment. At the onset of treatment, the fish were between 2.4 and 3.0 cm long. For the main study, two groups were used, each containing 10 animals. Ten Control fish were also included. Animals were placed in 84-liter glass tanks containing 50 liters of dechlorinated drinking water with an initial hardness of between 196.9 and 214.8 mg/l. The pH value was between 8.4 and 8.5 and temperature was between 19 and 22 °C. The dissolved oxygen concentration was maintained at between 70 and 95%. Feeding was stopped 24 hours before the test began. No food was offered during the period of exposure to the test substance. The test substance was administered in a single dose, dissolved in the water. There was no renewal of the test solution during the study period. After test initiation, fish were observed once daily for a total of 96 hours. Any dead animals found at the different observation times were

removed and their death was recorded. Animals showing no perceptible breathing movements and that did not react when the caudal fin was touched were considered dead. pH value dissolved oxygen level and temperature were recorded daily. Animals surviving to the end of the trial were sacrificed by asphyxia.

Results

Nominal concentrations (mg/l):	0 (control), 5.66 and 8
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
Element value:	
Statistical results:	LC_{50} = 6.73 mg/l
Remarks:	The 10 fish exposed to the 8.0 mg/l concentration died during the first 24 hours after treatment. Before death, they showed a decrease in mobility and breathing difficulties. Two of the animals remained on the surface of the aquarium and the others at the bottom. The 5.66 mg/l concentration did not cause the death of any of the treated animals. Only a slight decrease in mobility was noted between 3 and 24 hours after treatment. None of the fish in the Control group died. Values for pH ranged between 8.40 – 8.53, temperature ranged between 20.7 – 21.9 °C and dissolved oxygen values ranged between 70 and 94%. During the course of the study, the following deviations from the study protocol occurred: the pH value was sometimes up to 0.4 points higher and temperature 4 and 2 degrees lower than the ranges stated in the test protocol (pH 6.0 – 8.5 and temperature 21 – 25 °C).

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Mayordomo, L. 1992. Acute Toxicity Test. Determination of LC_{50} in Fish. (*Brachydanio rerio*). Test Substance: Betadet HR. Report number CD-91/2689T. Centro de Investigacion y Desarrollo Aplicado, s.a.l., Barcelona, Spain. Sponsored by Kao Corporation S.A.

Other Available Reports

Other

Last changed:	October 29, 2001
Order number for sorting:	157c
Remarks:	

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Test Substance

Identity:	Fatty acid C_{12-18} amido-propyl betain (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivatives, inner salt)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	OECD 204 Long Term Fish Test
Type:	Not stated
GLP:	Yes
Year:	1997 (date article was published)
Species/Strain/Supplier:	Rainbow trout (*Oncorhynchus mykiss)*
Analytical monitoring:	Yes
Exposure period:	28 days
Statistical methods:	Not stated
Remarks:	

Results

Nominal concentrations (µ/l):	Not stated
Measured concentrations: (µ/l)	Not stated
Unit:	mg/l
Element value:	NOEC and LOEC
Statistical results:	28-day NOEC = 0.16 mg/l 28-day LOEC = 0.5 mg/l
Remarks:	Manuscript indicates "biological data are backed by appropriate analytical determinations".

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions; guideline study summarized in a well-documented publication.

References

Scholz, N. 1997. Ecotoxicology of Surfactants. Tenside Surf. Det. (34)4:229 -232.

Other Available Reports

Other

Last changed: October 29, 2001
Order number for sorting: 157r
Remarks:

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivs., inner salt (CAS RN 61789-40-0)
Purity:	30% active ingredient; about 5% NaCl, about 65% water
Remarks:	

Method

Method/Guideline followed:	Methods conformed to OECD Guideline 202 and EEC Method C.2
Test type:	Static
GLP:	Yes
Year:	1991
Analytical procedures:	Yes
Species/Strain:	*Daphnia magna*
Test details:	Static
Statistical methods:	Logit model described by Cox, D. R. 1977. Analysis of binary data. Methuen & Co., Ltd.
Remarks:	The experiment measured the 48-hour acute toxicity of the test substance to *Daphnia magna*. The daphnids were exposed to the substance in 50-ml beakers containing 20 ml of test solution with 10 daphnids per beaker. Daphnids were laboratory bred and less than 24 hours old at test initiation. Test levels were 0 (control), 6.25, 12.5, 25, 50 and 100 mg/l. Test levels were run in duplicate. Dilution water was reconstituted water prepared according to the EEC Directive. The pH of the water was adjusted to 8.1 and the dissolved oxygen was 8.1 mg/l. During the test, pH ranged from 8.2 – 8.4 and dissolved oxygen ranged from 7.9 – 8.3. The concentration of the test article at the beginning and at the end of the test was analyzed for the control and for the 6.25, 25, and 100 mg/l test solutions. In addition, stability analyses gave values 95.5 and 85.2% of nominal for a 100 mg/l solution at the beginning and end of the test.

Results

Nominal concentrations (mg/l):	0 (control), 6.25, 12.5, 25, 50 and 100
Measured concentrations (mg/l):	0-hour measurements: < 1.235 (control), 4.515 (6.25 mg/l), 20.10 (25 mg/l nominal), 87.85 (100 mg/l nominal) mg/l 48-hour measurements: < 1.234 (control), 5.557 (6.25 mg/l nominal), 21.08 (25 mg/l nominal), 105.8 (100 mg/l nominal) mg/l

Unit:	mg/l
EC_{50} (48-hour):	21.5 mg/l (95% confidence limits: 16.1 – 28.1 mg/l)
NOEC (48-hour):	EC_0 = 5.3 mg/l
Statistical results:	Described above
Remarks:	Additional endpoints calculated during the test were: 24-h EC_0 = 12.5 mg/l 24-h EC_{50} = > 100 mg/l 24h EC_{100} = > 100 mg/l 48-h EC_0 = 5.3 mg/l 48-h EC_{50} = 21.5 mg/l 48-h EC_{100} = 89.3 mg/l Concentration analyses showed test levels remained from 72.2 to 105.8% of the nominal concentrations over the 48-hour test period. Daphnids in the control group showed no adverse effects during the exposure.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Wuethrich, V. 1991. 48-Hour Acute Toxicity of TEGO-BETAIN to *Daphnia magna* (OECD-Immobilization Test). Report number 283803. RCC Umweltchemie, Itingen/BL, Switzerland.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	87
Remarks:	

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Betadet HR (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivatives, inner salt)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Protocol number 202, part I, 24 h EC_{50} Acute Immobilization Test, of the 4th of April 1984, from the OECD Guideline for Testing of Chemicals
Test type:	Static
GLP:	Yes
Year:	1992
Analytical procedures:	No
Species/Strain:	*Daphnia magna*
Test details:	Static
Statistical methods:	Litchfield and Wilcoxon Method
Remarks:	The product was administered in a single dose per dose level, dissolved in the water held in the test tubes, which was similar to that used in the breeding period (50% dechlorinated water and 50% distilled water). The *daphnia* were then transferred to the vessels. The dilution water was aerated to saturation level prior to introduction of the test substance to ensure that the oxygen level did not fall below 60% of the saturation value. Before the Main Study, a Preliminary study was carried out to determine the range of toxic concentrations. The *Daphnia* were monitored one, 24 and 48 hours after the start of treatment. Observations included a determination of the number of immobilized animals, that is to say animals not able to swim within 15 seconds after gentle agitation of the test container.

Results

Nominal concentrations (mg/l):	0 (control), 0.5, 1, 2, 4, 8 and 16 mg/l
Measured concentrations (mg/l):	Not determined
Unit:	mg/l
EC_{50} (48-hour):	6.40 mg/l
Remarks:	48-hour EC_{50} = 6.40 mg/l (confidence limit 4.57 – 8.96). The product caused 0% immobilization at the 0.5 mg/l concentration. At concentrations of 1 mg/l and 2 mg/l, 2 and 3 daphnia, respectively, out of a total of 40, were found immobile. The 4 mg/l and 8 mg/l concentrations caused

immobilization in 5 and 9 daphnia, respectively, out of a total of 20. All the animals treated at the 16 mg/l concentration were found immobile. 1.7% immobilization was recorded in the Control group.
The following deviations from the test protocol occurred during the course of the study: during breeding, the temperature of the water was up to 1 degree and occasionally 2 degrees higher than the ranges stated the test protocol (20 ± 2 °C). Values for pH ranged from 8.33 – 8.49, temperature ranged between 21.9 – 22.4 °C and dissolved oxygen ranged between 67 – 100%.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1A
Remarks: Reliable without restriction; guideline study.

References

Mayordomo, L. and J. Zapatero. 1992. Acute Immobilisation Test in *Daphnia*. Test Substance: Betadet HR. Report number CD-91/2690T. Centro de Ivestigacion y Desarrollo Aplicado, s.a.l., Barcelona, Spain.

Other Available Reports

Other

Last changed: July 3, 2001
Order number for sorting: 157d
Remarks:

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Dehyton K, 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivs., hydroxides, inner salt (CAS RN 61789-40-0)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on microcrustaceans (Daphnia-Shorttime-Test) DIN 38412, L11. This test corresponds to OECD Guideline 202, part 1
Test type:	Static
GLP:	No
Year:	1980
Analytical procedures:	Not stated
Species/Strain:	*Daphnia magna*
Test details:	Static
Statistical methods:	Not stated
Remarks:	Organisms were exposed to the test substance added to water at a range of concentrations (approximately 20 animals per concentration) for a period of 24 hours. Immobilities (the loss of the ability to swim) were recorded and ultimately, the EC_0 and the EC_{100} were determined. Based on these data the EC_{50} was calculated.

Results

Nominal concentrations (mg/l):	Not stated
Measured concentrations (mg/l):	Not measured
Unit:	mg/l
EC_{50} (24-hour):	3.7 mg product/l (= 1.1 mg active matter/l)
LC_{50} (24-hour):	Not stated
NOEC (24-hour):	Corresponds to EC_0 (see below)
Statistical results:	Not stated
Remarks:	Also EC_0 (24 hour) = 2.2 mg product/l (= 0.64 mg active matter/l); EC_{100}(24 hour) = 6.4 mg product/l (= 1.9 mg active matter/l).

Conclusions

Remarks:	The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; data are reliable but article lacks details.

References

Steber, J. and K. Richterich. 2000. Acute Toxicity: *Daphnia*. Biological Research and Product Safety/Ecology: Unpublished Data, File 407/3. Henkel KGaA, Germany, Report No. R 0001217.

Other Available Reports

Other

Last changed:	July 3, 2001
Order number for sorting:	157p
Remarks:	

4.2 Toxicity to Aquatic Invertebrates

Test Substance

Identity:	Fatty acid C_{12-18} amido-propyl betain (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivatives, inner salt)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	OECD 202 *Daphnia* Reproduction Test
Test type:	Not stated
GLP:	Yes
Year:	1997 (date article published)
Analytical procedures:	Not stated
Species/Strain:	*Daphnia magna*
Test details:	Not stated
Statistical methods:	Not stated
Remarks:	

Results

Nominal concentrations (mg/l):	Not stated
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
EC_{50} (48-hour):	Not stated
LC_{50} (48-hour):	Not stated
NOEC (48-hour):	NOEC (21-day) = 0.9 mg/l
Statistical results:	Not stated
Remarks:	LOEC (21-day) = 3.6 mg/l; manuscript indicates "biological data are backed by appropriate analytical determinations".

Conclusions

Remarks:	The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions; guideline study summarized in a well-documented publication.

References

Scholz, N. 1997. Ecotoxicology of Surfactants. Tenside Surf. Det. (34)4:229 - 232.

Other Available Reports

Other

Last changed:	July 3, 2001
Order number for sorting:	157r
Remarks:	

4.2 TOXICITY TO AQUATIC INVERTEBRATES

Test Substance

Identity:	Ammonium, (carboxymethyl) hexadecyldimethyl-, hydroxide, inner salt (8CI) (CAS RN 693-33-4)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Nonspecific method
Test type:	Static
GLP:	No
Year:	1995
Analytical procedures:	No
Species/Strain:	*Echinogammarus tibaldii*
Test details:	Static
Statistical methods:	Probit analysis for EC_{50} concentrations
Remarks:	Test organisms were field collected from a spring of the Vera River (Italy) and held in the laboratory in cool aerated water in a 20-l aquaria. Mature adult males were kept for about three days in reconstituted water receiving aeration and food consisting of dry poplar leaves. Twenty-four hours before the test the feeding was ceased. Testing was conducted in 1-l glass jars containing 250 ml of test solution. Dilution water was reconstituted water having a hardness of 240 mg $CaCO_3$/l, an alkalinity of 55 mg $CaCO_3$/l and pH of 7.9. The temperature of the water during testing was 8 ± 0.5 °C. Animals were not fed during the test.

Results

Nominal concentrations (mg/l):	Not stated
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
EC_{50} (96-hour):	2.5 mg/l (95% confidence interval: 2.4 – 2.6 mg/l)
Remarks:	

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2C
Remarks:	Reliable with restrictions; comparable to guideline study with acceptable restrictions.

References

Pantani, C, N. Spreti , A. A. Novelli, A. V. Ghirardini and P. F. Ghetti. 1995. Effect of Particulate Matter on Copper and Surfactants' Acute Toxicity to *Echinogammarus tibaldii* (Crustacea, Amphipoda). Environ. Technol. 16:263 - 270.

Other Available Reports

Other

Last changed:	July 24, 2000
Order number for sorting:	59
Remarks:	

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	Cocamidopropyl Betaine – F 3006 (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivs., inner salt)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	OECD Guideline 201
Test type:	Static
GLP:	No
Year:	1993
Species/Strain/Supplier:	*Scenedesmus subspicatus*/CHODAT SAG 86.81/Not stated
Element basis:	Biomass and growth rate
Exposure period:	72 hours
Analytical monitoring:	No
Statistical methods:	Graphical determination of EC values
Remarks:	The study measured the inhibition of the test substance on the growth of *Scenedesmus subspicatus* over a 72-hour exposure period. Four replicate test flasks were run at each treatment level. Tests were run under continuous lighting of 35 – 70 $\mu E/m^2*s$ at a temperature of 23 ± 2 °C. Endpoints were determined for algal growth rate and algal cell density. The EC_0, EC_{10}, and EC_{50} were calculated for rate and cell density.

Results

Nominal concentrations (mg/l):	0 (control), 0.32, 1.0, 3.2, 10, 32, and 100 mg/l
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
Element value:	72-hour E_bC_{50} and 72-hour E_rC_{50}
Result:	72-hour E_bC_0 = 3.2 mg/l 72-hour E_bC_{10} = 4.9 mg/l 72-hour E_bC_{50} = 30 mg/l 72-hour E_rC_0 = 3.2 mg/l 72-hour E_rC_{10} = 7.0 mg/l 72-hour E_rC_{50} = 48 mg/l
Satisfactory control response:	Yes
Statistical results:	See Results
Remarks:	

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Noack, U. 1993. Pruefung auf Hemmung der Algenzellvermehrung von Cocamidopropyl Betaine – F 3006. Projekt Nr. 931124GG. Laboratorium fur Angewandte Biologie, Hildesheim, Germany.

Other

Last changed:	July 24, 2000
Order number for sorting:	91
Remarks:	

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivs., hydroxides, inner salt (CAS RN 61789-40-0)
Purity:	30% active substance
Remarks:	

Method

Method/Guideline followed:	DIN 38412, Part 9
Test type:	Static
GLP:	Yes
Year:	1992
Species/Strain/Supplier:	*Scenedesmus subspicatus*/SAG 8681/ Pflanzenphysiologisches Institut der Universitaet Goettingen
Element basis:	1×10^4 cells/ml
Exposure period:	96 hours
Analytical monitoring:	Not stated
Statistical methods:	Probit analysis of growth rate data
Remarks:	The experiment assessed the growth inhibition of the test substance on *Scenedesmus subspicatus*. Test concentrations were 0 (control), 0.01, 0.03, 0.1, 0.3, 1.0, 3.0 and 10 mg product/l. Each experimental group was replicated three times. Test vessels were 300-ml Erlenmeyer flasks holding 100 ml of test solution. At the beginning of the test, flasks were inoculated with 1.0 ml of algal cell inoculum to achieve a concentration in each flask of 1×10^4 cells/ml. Flasks were placed under continuous lighting of 2000 lux and continuously shaken at 120 rpm by means of an orbital shaker. At 24, 48, 72 and 96 hours, a sample from each flask was taken and the density of algal cells in the sample (cells/ml) was measured using an electronic particle counter (Coulter-Counter). Cell densities were converted to growth rates and growth rates were used in the calculation of EC values.

Results

Nominal concentrations (mg/l):	0 (control), 0.01, 0.03, 0.1, 0.3, 1.0, 3.0 and 10
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
Element value:	96-hour EC_{50}
Result:	96-hour EC_{50} = 1.84 mg product/l 96-hour EC_{50} = 0.55 mg active substance/l
Satisfactory control response:	yes

Statistical results:

Remarks: Additional endpoints determined in the study included:
96-hour EC_0 = 0.30 mg product/l
96-hour EC_0 = 0.09 mg active substance/l
96-hour EC_{10} = 0.46 mg product/l
96-hour EC_{10} = 0.14 mg active substance/l.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1B
Remarks: Reliable without restriction; comparable to guideline study.

References

H. Guhl. 1992. Forschung Biologie/Oekologie. Report number RE 920184. Henkel KGaA, Duesseldorf, Germany.

Other

Last changed: July 24, 2000
Order number for sorting: 93
Remarks:

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	TEGO®-Betain L 7 F (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivs., inner salt)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	OECD Guideline 201, bzw. Anhang zur Richtlinie 92/69 EWG Teil C.3
Test type:	Growth inhibition test
GLP:	Not stated
Year:	1995
Species/Strain/Supplier:	*Scenedesmus subspicatus*
Element basis:	Determined on cell biomass.
Exposure period:	72 hours
Analytical monitoring:	Not stated
Statistical methods:	Not stated
Remarks:	

Results

Nominal concentrations (mg/l):	Not stated
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
Element value:	72-hour EC_{50}
Result:	72-hour EC_{50} = 1.81 mg product/l 72-hour EC_{50} = 0.55 mg active substance/l
Satisfactory control response:	Unknown
Statistical results:	72-hour EC_{50} = 1.81 mg product/l 72-hour EC_{50} = 0.55 mg active substance/l
Remarks:	Additional endpoints determined in the study included: 72-hour EC_0 = 0.30 mg product/l = 0.09 mg active substance/l 72-hour EC_{10} = 0.46 mg product/l = 0.14 mg active substance/l

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Reliable with restrictions; basic information given; comparable to guidelines/standards.

References

1995. Algeninhibitionstest mit TEGO® Betain L 7 F. Report number bet7al. Th. Goldschmidt AG.

Other

Last changed:	July 24, 2000
Order number for sorting:	94b
Remarks:	

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	Fatty acid C_{12-18} amido propyl betain (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivatives, inner salt)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	EG 92/69 Algae Growth Inhibition Test
Test type:	Not stated
GLP:	Yes
Year:	1997
Species/Strain/Supplier:	*Scenedesmus subspicatus*/Not stated/Not stated
Element basis:	Not stated
Exposure period:	72 hours
Analytical monitoring:	Not stated
Statistical methods:	Not stated
Remarks:	

Results

Nominal concentrations (mg/l):	Not stated
Measured concentrations (mg/l):	Not stated
Unit:	mg/l
Element value:	72-hour NOEC
Result:	NOEC (72-hour) = 0.96 mg/l
Satisfactory control response:	Not stated
Remarks:	Manuscript indicates “biological data are backed by appropriate analytical determinations”.

Conclusions

Remarks:	The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2A
Remarks:	Reliable with restrictions; guideline study summarized in a well-documented publication.

References

Scholz, N. 1997. Ecotoxicology of Surfactants. Tenside Surf. Det. (34)4:229 - 232.

Other

Last changed:	July 3, 2001
Order number for sorting:	157r
Remarks:	

4.3 TOXICITY TO AQUATIC PLANTS (ALGAE)

Test Substance

Identity:	ANFODAC LB – alchil (C12) ammido propil betaina (CAS RN 4292-10-8; 1-Propanaminium, N-(carboxymethyl)-N,N-dimethyl-3-[(1-oxododecyl)amino]-, inner salt)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	EEC Directive 92/69 and OECD Guideline 201
Test type:	Static
GLP:	Not stated
Year:	1996
Species/Strain/Supplier:	*Selenastrum capricornutum prinz*/Institute of Terrestrial Ecology Culture Center of Algae and Protozoa, Cambridge, England
Element basis:	10^4 cells/ml
Exposure period:	72 hours
Analytical monitoring:	Not stated
Statistical methods:	The percentage difference between the cellular concentration of the treated group and the control group was calculated. The growth curve for both groups was graphically determined and the regression line was calculated. The difference between the average rate of growth (m) of treated and control groups was calculated by the angular coefficient (b) of the regression lines. The percentage inhibition of growth rate for each concentration of test material (Imt) was calculated as: Imt = [(mc-mt)/mc] x 100 where; mc = rate of growth of control group and mt = rate of growth of treated group.
Remarks:	A preliminary test to determine the acute toxicity of the test substance on an algal culture of Selenastrum capricornutum in growing phase, at an initial concentration of 10^4/ml was conducted. Algae were exposed to the test material at a concentration of 100 mg/l for 72 hours. The flasks containing the control and the treated organisms were stirred at a temperature of 23 ± 2 °C with continuous lighting for 72 hours. After 24, 48 and 72 hours, cell concentration was measured with a Burke chamber. The pH of the culture medium was 8.0 ± 0.5.

Results

Nominal concentrations (mg/l): 100 mg/l
Measured concentrations (mg/l): Not stated
Unit: mg/l
Element value:
Result: This was considered a "limit test". In this experiment, no difference in algal growth was seen between treated and control groups. The difference between the biomass of the control and treated groups is less than 25%. The difference between the average growth of the treated group and control group was 0.56%. The NOEC was 100 mg/l.
Satisfactory control response: Yes
Statistical results: Not stated
Remarks: The temperature during the test did not vary more than 1 °C and the pH did not vary more than 0.2 units. The average cellular concentrations for each group were:

Time (hours)	Treated (no. cells/ml)	Control (no. cells/ml)	Difference (%)
24	2.7×10^4	2.5×10^4	-8.0
48	5.3×10^4	5.5×10^4	3.6
72	8.7×10^4	8.5×10^4	-2.3

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1A
Remarks: Reliable without restriction; guideline study.

References

Biffi E. 1996. Acute Toxicity in Algae: Test Material: ANFODAC LB. Unpublished Report (Project number 96/200.A7) Biolab, Italy.

Other

Last changed: July 3, 2001
Order number for sorting: 167
Remarks:

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Amphosol CA (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivs., inner salt)
Purity:	35.61% active
Remarks:	

Method

Method/guideline followed:	Not stated
Type:	LD_{50}
GLP:	Yes
Year:	1982
Species/Strain:	Rats/Sprague-Dawley
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Oral gavage
Remarks:	Five male and five female rats (220 - 294 g) were administered a single oral dose of the undiluted test substance. Animals were fasted overnight prior to dosing. All animals were weighed prior to dosing and at termination. Animals were observed frequently on the day of dosing and for 14 days subsequent to dosing. All animals that died during the study were subjected to a gross necropsy.

Results

Value:	LD_{50} > 1.8 g/kg for males (since all females died could not determine LD_{50} for females or determine a combined LD_{50})
Number of deaths:	5 of 10
Remarks:	All five females died by Day 2 (one day after dosing). All females exhibited salivation, diarrhea, ataxia, and/or decreased activity prior to death. The males exhibited similar clinical signs as the females on Days 1 (day of dosing) and 2; however, all animals recovered by Day 3. Necropsy data were not reported.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1B
Remarks:	Reliable without restriction; comparable to guideline study.

References

Reagan, E. L. and P. J. Becci. Acute Oral Toxicity in Rats. 1982. Study number 7330D. Food and Drug Research Laboratories, Inc., Waverly, NY, U. S.

Other Available Reports

Other

Last changed:	July 25, 2000
Order number for sorting:	99a
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Lonzaine Co. Lot #B-4232 (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivs., inner salt)
Purity:	30%
Remarks:	Remaining composition is 70% water

Method

Method/guideline followed:	Acute toxicity procedure suggested in: Hagan, E. C. 1959. Acute Toxicity; Appraisal of the safety of chemicals in foods, drugs and cosmetics. 17 – 25.)
Type:	LD_{50}
GLP:	No
Year:	1977
Species/Strain:	Wistar rats
Sex:	Male and female
No. of animals per dose:	5
Vehicle:	None
Route of administration:	Oral gavage
Remarks:	Six groups of five young adult albino rats (males and females combined) weighing 200 – 300 g were administered a single dose of the test substance (30% aqueous solution) at levels of 4.0, 8.0, 10.0, 12.5, 16.0 or 32.0 g/kg. The test substance was used as received. Animals were fasted for 24 hours prior to dosing and both sexes were equally distributed. Animals were observed daily for two weeks post-dose. No postmortem, or histopathology examinations were performed in this study.

Results

Value:	LD_{50} = 2.6 g active ingredient/kg (95% Confidence Limits = 1.8 – 3.6 g active ingredient/kg)
Number of deaths:	0/5 at 4.0 g/kg dose level (original solution) 2/5 at 8.0 g/kg dose level (original solution) 4/5 at 10.0 g/kg dose level (original solution) 5/5 at 12.5, 16.0 and 32.0 g/kg dose levels (original solution)
Remarks:	Slight diarrhea and unkempt coats were observed in animals treated with 4.0 g/kg of the test substance as an aqueous mixture. Lethargy, diarrhea, nasal hemorrhage and unkempt coats, increasing in severity proportionately to the levels employed, were observed in all animals treated at

dose levels of 8.0 g/kg (test substance as an aqueous mixture) and above.
The LD_{50} of the original solution (30% aqueous) was 8.55 g/kg.

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2B
Remarks: Reliable with restrictions; basic data given, comparable to guidelines/standards.

References

Wallace, J. M. 1977. Acute Oral LD_{50} Toxicity Study with Lonzaine CO, Lot #B-4232. Bio-Toxicology Laboratories, Inc., Moorestown, NJ, U. S.

Other Available Reports

Other

Last changed: August 14, 2000
Order number for sorting: 99c
Remarks:

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Cocamidopropyl Betaine (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivs., inner salt)
Purity:	30%
Remarks:	Remaining composition is 70% water

Method

Method/guideline followed:	Acute toxicity procedure suggested in: Hagan, E. C. 1959. Acute Toxicity; Appraisal of the safety of chemicals in foods, drugs and cosmetics. 17 – 25.)
Type:	LD_{50}
GLP:	No
Year:	1977
Species/Strain:	Wistar rats
Sex:	Male and female
No. of animals per dose:	5
Vehicle:	None
Route of administration:	Oral gavage
Remarks:	Six groups of five young adult albino rats (males and females combined) weighing 200 – 300 g, were administered a single dose of the test substance (30 % aqueous solution) at levels of 2.0, 4.0, 5.0, 6.3, 8.0 or 16.0 g/kg. The test substance was used as received. Animals were fasted for 24 hours prior to dosing and both sexes were equally distributed. Animals were observed daily for two weeks post-dose. No postmortem, or histopathology examinations were performed in this study.

Results

Value:	LD_{50} = 1.5 g active ingredient/kg (95% Confidence Limits = 1.1 – 2.0 g/kg)
Number of deaths:	0/5 at 2.0 g/kg dose level (original solution) 1/5 at 4.0 g/kg dose level (original solution) 2/5 at 5.0 g/kg dose level (original solution) 3/5 at 6.3 g/kg dose level (original solution) 5/5 at 8.0 and 16.0 g/kg dose levels (original solution)
Remarks:	Sluggishness, nasal hemorrhage, diarrhea and wetness around the posterior, increasing in severity proportionately to the levels employed, were observed in animals at all dose levels. The LD_{50} of the original solution (30%) was 4.9 g/kg.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2B
Remarks:	Reliable with restrictions; basic data given, comparable to guidelines/standards.

References

Wallace, J. M. 1977. Acute Oral LD_{50} Toxicity Study for Cocamidopropyl Betaine 30% Solution. Bio-Toxicology Laboratories, Inc., Moorestown, NJ, U. S.

Other Available Reports

Other

Last changed:	August 14, 2000
Order number for sorting:	99d
Remarks:	

5.1.1 ACUTE ORAL TOXICITY

Test Substance

Identity:	Betadet HR (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivatives, inner salt)
Purity:	31% active ingredient
Remarks:	

Method

Method/guideline followed:	Annex V of EEC directive 79/831/EEC, Part B Methods for Determination of Toxicity, Method B1 Acute Oral Toxicity and OECD Guideline for Testing of Chemicals Number 401.
Type:	LD_{50} limit test
GLP:	Not stated
Year:	1987
Species/Strain:	CD rats [Crl:COBS CD (SD) BR]
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	Not stated
Route of administration:	Oral
Remarks:	The study was performed on male and female CD rats whose body weights ranged between 110 and 150 g. The test substance was administered as provided at 5.0 g/kg body weight via syringe and plastic catheter. Animals were observed soon after dosing and at frequent intervals for the remainder of Day 1. On subsequent days, the animals were observed once in the morning and again at the end of the experimental day. Clinical signs were recorded at each observation. All animals were observed for 14 days after dosing. Individual body weights were recorded on days 1, 8 and 15. All animals were killed on Day 15 by cervical dislocation and were subjected to a macroscopic post mortem examination, which consisted of opening the abdominal and thoracic cavities. The macroscopic appearance of abnormal organs, when present, was recorded.

Results

Value:	LD_{50} > 1.5 g/kg active ingredient (> 5.0 g/kg as supplied – 31% solution)
Number of deaths:	None
Remarks:	Signs of reaction to treatment observed in all rats shortly after dosing were: piloerection and increased salivation.

Piloerection persisted throughout Day 1 and was accompanied on Day 2 by abnormal body carriage (hunched posture) and diarrhea. Recovery, as judged by external appearance and behavior, was advanced by Day 3 (piloerection alone) and complete by Day 4. Slightly low body weight gains were recorded for four males and three females on Day 8. All rats achieved anticipated body weight gains during the second week of the study. Terminal autopsy findings were normal. The acute lethal oral dose to rats of Betadet HR was found to be greater than 5.0 g/kg body weight of the 31% solution (> 1.5 g/kg active ingredient).

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1A
Remarks: Reliable without restriction; guideline study.

References

Gardner, J. R. 1987. Acute Oral Toxicity to Rats of Betadet HR. Report number 871209D/MLS 5/AC. Huntingdon Research Centre Ltd., Cambridgeshire, UK, Sponsored by Kao Corporation S.A.

Other available reports

Other

Last changed: July 3, 2001
Order number for sorting: 157h
Remarks:

5.1.3 ACUTE DERMAL TOXICITY

Test Substance

Identity:	Betadet HR (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivatives, inner salt)
Purity:	31% active ingredient
Remarks:	

Method

Method/guideline followed:	Annex V of EEC directive 79/831/EEC, Part B methods for Determination of Toxicity Method B3 Acute Dermal Toxicity and the OECD Guideline for Testing of Chemicals Number 402.
Type:	LD_{50} limit test
GLP:	Not stated
Year:	1987
Species/Strain:	CD rats [Crl:COBS CD (SD) BR]
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	Not stated
Route of administration:	Dermal
Remarks:	The study was designed to assess the toxicity following a single dermal dose of the test substance. The animals were in a weight range of 200 to 232 g prior to dosing. The rats were treated at 2.0 g/kg bodyweight. One day prior to treatment, hair was removed from the dorsolumbar region of each rat with electric clippers exposing an area equivalent to 10% of the total body surface. No shaving or chemical depilation was used. The test substance was applied by spreading it evenly over the prepared skin. The treated area was then promptly covered with gauze, which was held in place with an impermeable dressing encircled firmly around the trunk. At the end of the 24-hour exposure period, the dressings were carefully removed and the treated area of skin decontaminated by washing in warm (30 - 40 °C) water and blotting dry with absorbent paper. The treated areas of skin were examined daily for 14 days for signs of dermal irritation and assessed according to an arbitrary scoring system. Individual body weights of rats in the study were recorded on Days 1, 8 and 15. All animals were killed on Day 15 by cervical dislocation and were subjected to a macroscopic post mortem examination, which consisted of opening the

abdominal and thoracic cavities. The macroscopic appearance of abnormal organs when present was recorded.

Results

Value:	> 2 g/kg
Number of deaths:	None
Remarks:	The acute lethal dermal dose to rats of Betadet HR was found to be greater than 2.0 g/kg body weight. There were no deaths following a single dermal dose of Betadet HR at 2.0 g/kg body weight. There were no clinical signs of systemic reaction t to treatment. Sites of application of the test substance showed slight or well-defined erythema on Day 2. Well-defined erythema persisted in three male and all female rats on Day 3. There were no more intense reactions to treatment, and resolution of erythema was completed by Day 6. Slough or hyperkeratinization affected the treated skin of 4, 5, 6, 8, 9 and 10 rats on Days 4 and 5 only. Terminal autopsy findings were normal.

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Gardner, J. R. 1987. Acute Dermal Toxicity to Rats of Betadet HR. Report number 871210D/MLS 6/AC. Huntingdon Research Centre Ltd., Cambridgeshire, UK, Sponsored by Kao Corporation S.A.

Other

Last changed:	July 3, 2001
Order number for sorting:	157i
Remarks:	

5.4 REPEATED DOSE TOXICITY

Test Substance

Identity:	Tego® Betain (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivs., inner salt)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	OECD Method No. 408
Test type:	Oral
GLP:	Yes
Year:	1991
Species:	Rat
Strain:	Crl:CF®(SD)BR Sprague Dawley
Route of administration:	Oral gavage
Duration of test:	92 days
Doses/concentration levels:	250, 500 and 1000 mg/kg/day
Sex:	Male and female
Exposure period:	92 days
Frequency of treatment:	One daily dose
Control group and treatment:	Yes (concurrent, treated with distilled water)
Postexposure observation period:	None
Statistical methods:	For body weight and food consumption data, the Levene's test for homogeneity of variances was performed followed by one-way ANOVA. If the ANOVA was significant, the Dunnett's test for multiple group comparisons was performed. For organ weights, the ANOVA was performed with one factor, treatment, followed by the Student-Newman-Keuls test. For clinical chemistry, hematology and organ/body eight ratio data, the ANOVA was performed with one factor, treatment – based on taking the ranks of the variables – followed by the Student-Newman-Keuls test. Statistical evaluation was performed with the software package SAS (Statistical Analysis System).
Remarks:	Ten male (115 to 174 g) and 10 female rats (97 to 174 g), five to six weeks of age, were used on study. The test substance was administered in the vehicle, distilled water, at concentrations of 250, 500 and 1000 mg/kg body weight per day for 92 days. The dose volume was 10 ml/kg/day. Clinical signs were recorded at least daily. Body weight and food consumption were recorded once weekly. Ophthalmic examinations were recorded on the control and

1000 mg/kg/day animals prior to dosing and on all animals in all groups during the final week of treatment. Blood and urine samples were collected from all animals during the final week of treatment for hematological and biochemical investigations. Blood was collected from orbital sinus and urine was collected by placing animals in metabolism cages. Complete necropsy was performed on all surviving animals following 92 days of treatment. The following organs were weighed: adrenals, brain, heart, kidneys, liver, ovaries, pituitary, spleen, testes and thyroids (with parathyroids). Histopathology was performed on select tissues from all animals in the control group and the 1000 mg/kg/day group. Due to treatment-related histopathological changes seen in the 1000 mg/kg/day animals, stomach tissue of the 500 and 250 mg/kg/day groups were also examined microscopically.

Results

NOAEL (NOEL)	NOEL = 250 mg/kg/day
LOAEL (LOEL)	Not stated
Actual dose received:	250, 500 and 1000 mg/kg/day
Toxic response/effects:	Described below
Statistical results:	A few statistically significant differences were observed in clinical chemistry parameters between the tested groups; however, none were treatment-related. No other statistical results were stated.
Remarks:	There were no compound-related deaths. One control group male, one male and one female in the 500 mg/kg group and 3 females in the 1000 mg/kg group died accidentally. Throughout the experimental period, there were no treatment-related effects for either sex in the following parameters: clinical observations, body weight gain, food consumption, ophthalmic observations, hematologic evaluations, blood chemistry, urinalysis and organ weights. The macroscopic necropsy findings revealed some stomach ulceration at the fundus and cardiac regions in one high dose male and one high dose female. There were no other treatment-related macroscopic findings. Microscopic post-mortem findings revealed forestomach gastritis in six male and three female rats in the 1000 mg/kg/day group, and in two male and two females in the 500 mg/kg/day dose group. Forestomach gastritis was not present in the stomachs of the animals in the 250 mg/kg/day group. There was no evidence of any

systemic toxicity due to the test substance administration in any of the other organs examined.
Reproductive organs were examined histologically, thus this study meets the SIDS requirements for a reproductive screen.

Conclusions

Remarks: On the basis of the results obtained from this study, Tego Betain was very well tolerated at a dose level of 250 mg/kg/day, relatively well tolerated at a dose level of 500 and moderately tolerated at a dose level of 1000 mg/kg/day when administered daily by oral gavage to rats for a minimum of 90 days. The only signs of intolerance at the 500 and 1000 mg/kg/day dose level were a dose-related incidence of forestomach gastritis (author of the report).
The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1A
Remarks: Reliable without restriction; guideline study.

References

Zuehlke, U. 1991. 90 Day Oral (Gavage) Subchronic Toxicity Study in the Rat. Report number 954-348-155. Hazleton Laboratories Deutschland GmbH, Muenster, Germany.

Other

Last changed: June 24, 2004
Order number for sorting: 101
Remarks:

5.4 REPEATED DOSE TOXICITY

Test Substance

Identity:	Dehyton K (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivs., inner salt)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	Guideline 87/302/EWG Part B
Test type:	Oral gavage
GLP:	Yes
Year:	1991
Species:	Rat
Strain:	Sprague-Dawley
Route of administration:	Oral gavage
Duration of test:	28 days
Doses/concentration levels:	250, 500 and 1000 mg/kg body weight
Sex:	Male and female
Exposure period:	28 days
Frequency of treatment:	Once per day; 5 consecutive days per week
Control group and treatment:	Yes (concurrent, received distilled water)
Postexposure observation period:	28 days
Statistical methods:	T-test and Steel-Test (a multiple comparison rank sum test)
Remarks:	An additional 5 male and 5 female rats were included in the control and 1000 mg/kg levels to be used as a recovery group. Doses were adjusted to body weight.

Results

NOAEL (NOEL)	500 mg/kg/day
LOAEL (LOEL)	1000 mg/kg/day
Actual dose received:	Not stated
Toxic response/effects:	Described below
Statistical results:	Not stated
Remarks:	All doses were tolerated without substance-related lethality. Symptoms of local irritation of the gastrointestinal tract (head protrusion at the beginning of week 3, salivation at the beginning of week 4) were observed in the 1000 mg/kg group to the end of the study. No compound-related decreases in food consumption or water consumption were noted throughout the study. The hematological evaluations, clinical chemistry, ophthalmic examinations, and absolute and relative organ weighted showed no compound-related affects. The macroscopic examination

indicated compound-related edema of the mucosa of the forestomach in the 1000 mg/kg group. This finding of forestomach irritation disappeared in the male and female rats of the recovery group, 28 days after termination of treatment. Microscopic examination of the forestomach of the male and female rats in the high dose group showed effects indicating local irritation including acanthosis of the mucosa, inflammatory edema of the submucosa and multiple ulcerations. The acanthosis and the papillomatous hyperplasia were the dominant findings and were higher graded in the females than in the males. These were considered to be the result of the irritating property of the test substance and not to be symptoms of a systemic toxicity. The 1000 mg/kg recovery animals showed complete and regular regeneration of the forestomach mucosa. Microscopic examination revealed no lesions in the reproductive organs of the high-dose group male and female rats.

Conclusions

Remarks: According to the described study, a daily administration of Dehyton K up to 1000 mg/kg body weight does not cause cumulative systemic toxicity to rats (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1A
Remarks: Reliable without restrictions; Guideline study

References

Potokar, M., W. Sterzel and W. Pittermann. 1991. Dehyton K, 28-Tage-Test mit Wiederholter Oraler Verabreichung an Ratten. Report number TED 910119. Henkel KGaA, Duesseldorf, Germany.

Other

Last changed: June 24, 2004
Order number for sorting: 102a
Remarks:

5.4 REPEATED DOSE TOXICITY

Test Substance

Identity:	Cocamidopropyl betaine (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivs., inner salt)
Purity:	100%
Remarks:	

Method

Method/guideline followed:	Other
Test type:	Oral range-finding
GLP:	Yes
Year:	1988
Species:	Rat
Strain:	Sprague-Dawley
Route of administration:	Oral gavage
Duration of test:	7 days
Doses/concentration levels:	300, 650, 1000, 1500 and 3000 mg/kg/day
Sex:	Male and female
Exposure period:	7 days
Frequency of treatment:	One daily dose
Control group and treatment:	None
Postexposure observation period:	None
Statistical methods:	None
Remarks:	Two rats/sex/group were administered the undiluted test substance at doses of 300, 650, 1000, 1500 or 3000 mg/kg/day by oral gavage for seven days. Males (225 - 255.9 g) and females (241.5 - 266.9 g) approximately 8 and 12 weeks of age, respectively, were used on study. Animals were acclimated to the testing facility for approximately one week prior to test administration. Mortality/morbundity checks were performed twice daily. Observations for signs of toxic and pharmacologic effects were performed 1 to 2 hours post-dose for 7 days. Body weights were recorded immediately prior to initiation of dosing, at day 7, and at death or terminal sacrifice. Necropsies were performed on all animals. The study was designed as a range-finding study to determine dose levels for a 28-day study.

Results

NOAEL (NOEL):	Not stated
LOAEL (LOEL):	300 mg/kg/day
Actual dose received:	300, 650, 1000, 1500 and 3000 mg/kg/day

Toxic response/effects:	Described below
Statistical results:	None
Remarks:	All animals treated with the test substance at a dose level of 3000 mg/kg died by Day 4. One female in the 1500 mg/kg dose level died by Day 7 and the other female in this group showed dramatic weight loss. All animals in the 1000 and 300 mg/kg dose groups survived until study termination. One male in the 650 mg/kg dose group died; however, since no other animals died in this dose level nor at 1000 mg/kg, it was considered incidental. Clinical signs observed in females in the 300 mg/kg dose group included compound-colored urine, soft feces and nasal discharge. Males in this group appeared normal throughout the study. Compound-colored urine was observed in animals in all other dose groups. All animals treated with 3000 mg/kg showed signs of soft feces and depression prior to death. Marked body weight depression was seen in one 300 mg/kg group female, both 650 mg/kg group females, both 1000 mg/kg males and one 1500 mg/kg female. The remainder of animals that survived to termination gained weight. Pathological observations noted in animals that were found dead that appeared to be treatment related included dark liver, thin walls in the stomach and intestines, compound-like material in the stomach and intestines and distended intestines. All other observations were considered incidental in nature.

Conclusions

Remarks:	Based on the results of this range-finding study, a dose level of 1000 mg/kg/day is considered the highest recommended dose level acceptable for a 28-day study (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1B
Remarks:	Reliable without restriction; comparable to guideline study.

References

Bailey, D. E. 1988. Dose Range-finding Toxicity Study in Rats. Report number 444-223. Hazleton Laboratories America, Inc., Vienna, VA, U. S.

Other

Last changed:	July 27, 2000
Order number for sorting:	102b
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Dehyton K (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivs., inner salt)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	OECD Method No. 471 (May 26, 1983)
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Yes
Year:	1988
Species/Strain:	*Salmonella typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of Aroclor 1254-induced male rats
Concentrations tested:	1, 4, 16, 64 and 256 µg/plate (without S-9 activation) 4, 16, 64, 256 and 1024 µg/plate (with S-9 activation)
Statistical methods:	Not stated
Remarks:	Three plates per dose level. S-9 was purchased from an outside source. S-9 Mix was prepared on the day of the experiment. Double deionized water was used as the solvent and negative control substance. The plate incorporation method was used. An initial toxicity assay was performed at doses of 8, 40, 200, 1000 and 5000 µg/plate.

Results

Result:	Negative
Cytotoxic concentration:	In the initial toxicity assays, the test substance without metabolic activation was cytotoxic to the tester strains TA 1535 and TA 1537 at 1000 µg/plate and cytotoxic to tester strain TA 1538 at 200 µg/plate. The test substance with metabolic activation was cytotoxic to the tester strains TA 1535 and TA 1538 at 5000 µg/plate and tester strain TA 1537 at 1000 µg/plate.
Genotoxic effects:	Negative with and without activation
Statistical results:	None
Remarks:	

Conclusions

Remarks:	Dehyton K did not induce reverse mutations in the presence and absence of S-9 mix in the tester strains TA 1535, TA 100, TA 1537, TA 1538 and TA 98 (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Banduhn, N. 1991. Dehyton K, Prüfung auf Mutagenität im Ames-Test. Report number 880078. Henkel KGaA, Duesseldorf, Germany.

Other

Last changed:	August 14, 2000
Order number for sorting:	104
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Cocamidopropyl Betaine (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivs., inner salt)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	OECD Guideline No. 471
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Not stated
Year:	1995
Species/Strain:	*Salmonella typhimurium*/Not stated
Metabolic activation:	With and without S-9 activation
Concentrations tested:	Not stated
Statistical methods:	Not stated
Remarks:	

Results

Result:	Negative
Cytotoxic concentration:	Not stated
Genotoxic effects:	Negative with and without activation
Statistical results:	Not stated
Remarks:	

Conclusions

Remarks:	The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2D
Remarks:	Reliable with restrictions; summary of German article.

References

Gentoxizitaet (Rueckmutationsversuch/Amestest) mit TEGO® Betain L 7 F. 1995. Report number bet7ge. Th. Goldschmidt AG.

Other

Last changed:	July 25, 2000
Order number for sorting:	105a
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Cocamidopropyl Betaine (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivs., inner salt)
Purity:	30%
Remarks:	

Method

Method/guideline followed:	Techniques described in: Ames, B. N., J. McCann and E. Yamasaki. Methods for detecting carcinogens and mutagens with the *Salmonella*/mammalian microsome mutagenicity test. Mutat. Res. 31:347 - 364.
Type:	Reverse mutation assay
System of testing:	Bacterial
GLP:	Yes
Year:	1988
Species/Strain:	*Salmonella typhimurium* strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of Arochlor 1254-induced rats. S-9 mix was purchased commercially and was prepared fresh just prior to use in the assays.
Concentrations tested:	0.001, 0.005, 0.00, 0.050, 0.100, 0.125, 0.150 and 0.300 µl per plate
Statistical methods:	None performed
Remarks:	Three plates per dose level. The entire assay was performed once. Deionized water was used as the solvent in this test.

Results

Result:	The range finding study results indicated that the test substance was toxic towards the tester strains at 0.146 µl and higher. In the main study, no substantial increases in the revertant colony numbers of any of the five strains tested were observed following treatment with the test substance at any dose level, either in the presence or absence of S-9 activation.
Cytotoxic concentration:	0.586 µl per plate and above (based on range-finding study)
Genotoxic effects:	0.146 µl per plate and above (based on range-finding study) Negative with and without activation in the main study
Statistical results:	None
Remarks:	

Conclusions

Remarks:	The test substance, Cocamidopropyl Betaine, did not exhibit genetic activity in these assays and was not mutagenic under the test conditions according to the study criteria (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	2C
Remarks:	Reliable with restrictions; comparable to guideline study with acceptable restrictions.

References

Jagannath, D. R. 1988. Mutagenicity Test on Cocamidopropyl Betaine in the Ames Salmonella/Microsome Reverse Mutation Assay. Study number 10245-0-401. Hazleton Laboratories America, Inc., Kensington, MD, U. S.

Other

Last changed:	July 26, 2000
Order number for sorting:	105b
Remarks:	

5.5 GENETIC TOXICITY *IN VITRO*

Test Substance

Identity:	Betadet HR (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivatives, inner salt)
Purity:	28.5-30.5 % active ingredient
Remarks:	

Method

Method/guideline followed:	OECD Guidelines for the Testing of Chemicals, Protocol Number 471 and also Method B14 in commission directive 92/69/EEC
Type:	Ames
System of testing:	Bacterial
GLP:	Yes
Year:	1996
Species/Strain:	*Salmonella typhimurium* TA1535, TA1537, TA1538 and TA98
Metabolic activation:	With and without S-9 activation; S-9 mix obtained from the liver of Arochlor 1254-induced male Sprague-Dawley rats
Concentrations tested:	0, 50, 150, 500, 1500 and 5000 µg per plate
Statistical methods:	UKEMS (5) and Dunnett's Method of Linear Regression
Remarks:	In this assay, overnight sub-cultures of the appropriate coded stock cultures were prepared in nutrient broth and incubated at 37 °C for approximately 10 hours. S9 was prepared in-house from the livers of male Sprague-Dawley rats. A known aliquot of S9-mix and 2 ml of molten, trace histidine supplemented media were overlaid onto a sterile Vogel-Bonner Minimal agar plate in order to assess the sterility of the S9-mix. This procedure was repeated, in triplicate, on the day of each experiment. A preliminary test was carried out to determine the toxicity of the test material to the tester organisms. Two main studies were run. In the first main study up to six concentrations of the test material (1.5, 5, 15, 50 150 and 500 µg/plate) plus a control were assayed in triplicate against each tester strain, using the direct plate incorporation method in accordance with the standard methods for mutagenicity tests using bacteria. The second experiment was performed using methodology as described for experiment 1, using fresh bacterial cultures, with up to seven concentrations of test material (0.5, 1.5, 5, 15, 50, 150 and 500 µg/plate) and control solutions in triplicate. Both tests were run with and without metabolic activation. The following positive

controls were included in each test: N-ethyl-N'-nitro-N-nitrosoguanidine (3 µg/plate for TA100 and 5 µg/plate for TA 1535); 9-aminoacridine (80 µg/plate for TA1537); 4-nitro-o-phenylenediamine (5 ug/plate for TA1538); 4-nitroquinoline-1-oxide (0.2 ug/plate for TA98). In addition, the material, 2-aminoanthracene, which is non-mutagenic in the absence of metabolizing enzymes was used in the activated series (1 ug/plate for TA100, 2 ug/plate for TA1535 and TA1537, and 0.5 ug/plate for TA1538 and TA98). All of the plates were incubated at 37 °C for approximately 48 hours and the frequency of revertant colonies assessed using a Domino colony counter. The criteria for a substance to be considered positive in this test system were: a dose-related and statistically significant increase in mutation rate in one or more strains of bacteria in the presence and/or absence of the S9 microsomal enzymes in both experiments at sub-toxic dose levels. To be considered negative, the number of induced revertants compared to spontaneous revertants was less than twofold at each dose level employed, up to the limits imposed by toxicity, solubility or up to the maximum recommended dose of 5000 µg/plate. In this case the limiting factor was either toxicity or the maximum recommended dose depending upon bacterial strain type and presence or absence of S9-mix.

Results

Result:	Negative with and without activation.
Cytotoxic concentration:	150 ug/plate
Genotoxic effects:	None
Statistical results:	See below
Remarks:	The test material caused a visible reduction in the growth of the bacterial lawn to all of the strains tested. The first evidence of toxicity was observed at 150 µg/plate. No significant increase in the frequency of revertant colonies of bacteria was recorded for any of the strains used, at any dose level with or without metabolic activation. All of the positive control chemicals used in the test produced marked increases in the frequency of revertant colonies and the activity of the S9 fraction was found to be satisfactory.

Conclusions

Remarks:	The test material was found to be non-mutagenic under the conditions of this test. The endpoint has been adequately

characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1A
Remarks:	Reliable without restriction; guideline study.

References

Thompson, P. W. 1996. Betadet HR: Reverse Mutation Assay "Ames Test" Using *Salmonella typhimurium*. Project number 140/473. Safepharm Laboratories Limited, Derby, UK, Sponsored by Kao Corporation S.A.

Other

Last changed:	July 3, 2001
Order number for sorting:	157j
Remarks:	

5.6 GENETIC TOXICITY *IN VIVO*

Test Substance

Identity:	Tego Betain L7, batch 9775 (CAS RN 61789-40-0; 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivatives, hydroxides inner salt)
Purity:	Not stated
Remarks:	

Method

Method/Guideline followed:	Not stated
Type:	Mouse Micronucleus Test (Schmid Method)
GLP:	Yes
Year:	1987
Species:	Mouse
Strain:	OF1 (I.O.P.S. Caw)
Sex:	Male and female
Route of administration:	Intraperitoneal injection
Doses/concentration levels:	0.02 and 0.2 g/kg
Exposure period:	Two administrations at 24-hour intervals
Statistical methods:	Student's Test and Exact Bilateral Comparison Test
Remarks:	The purpose of the study was to evaluate the mutagenic potential of the test article in an in-life test that enabled detection of chromosomal mutations. Groups of five male and five female mice were administered two doses of the test substance by intraperitoneal injection in sterile distilled water at 24-hour intervals. Concentrations were 0.02 and 0.2 g/kg at a constant volume of 10 g/kg. Two additional groups of mice (five males and five females per group) were used as the vehicle control (sterile distilled water) and the positive control (cyclophosphamide, 0.1 g/kg). Animals were killed by cervical dislocation 6 hours after the second administration. The bone marrow was extracted from the femurs using fetal calf serum centrifuged and re-suspended. For each animal, two smears were prepared, air-dried and stained with freshly filtered May Grunwald and Giemsa staining. For each animal the reading was carried out by observation of 1000 polychromatic erythrocytes.

Results

Mitotic index: The results are expressed as the number of cells with micronuclei for each 1000 polychromatic erythrocytes observed.

Male mice	
Dose group	**Mean Number of Micronucleated Erythrocytes**
Negative Control	1.4
Positive Control	67.8
0.02 g/kg	0.8
0.2 g/kg	1.2

Female Mice	
Dose group	**Mean Number of Micronucleated Erythrocytes**
Negative Control	1.8
Positive Control	44.8
0.02 g/kg	1.6
0.2 g/kg	1.0

Male and Female Mice	
Dose group	**Mean Number of Micronucleated Erythrocytes**
Negative Control	1.6
Positive Control	56.3
0.02 g/kg	1.2
0.2 g/kg	1.1

Genotoxic effects: Negative
NOAEL (NOEL): > 0.2 g/kg
Statistical results: Described below
Remarks: No significant increase in the number of micronucleus-bearing erythrocytes was observed following two intraperitoneal administrations of the test substance. The results for each treated group were comparable with those obtained for the negative control group. The results obtained with cyclophosphamide positive control (100 mg/kg) are significantly positive. Under these conditions, it can be concluded that the test article induced no mutagenic effect in the mouse at dose levels of 0.02 and 0.2 g/kg.

Conclusions

Remarks:	The endpoint has been adequately characterized. (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch):	1B
Remarks:	Reliable without restriction; comparable to guideline study.

References

Weill, N. 1987. Tego Betain L7, Batch 9775: Micronucleus Test (Schmid Method). Report number 703201. Hazleton-IFT, St Germain sur l'Arbresle, France.

Other

Last changed:	July 3, 2001
Order number for sorting:	157k
Remarks:	

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Test Substance

Identity:	1-Hexadecanaminium (CAS RN 693-33-4; Ammonium, (carboxymethyl) hexadecyldimethyl-, hydroxide, inner salt)
Purity:	Not stated
Remarks:	

Method

Method/guideline followed:	None – pilot study
GLP:	Yes (FDA)
Year:	1984
Species:	Rabbits
Strain:	New Zealand White
Route of administration:	Dermal
Doses/concentration levels:	0, 10, 20, 40, 100 and 200 mg/kg/day
Sex:	Female
Exposure period:	Days 6 - 18 of gestation, except in 100 and 200 mg/kg/day dosage groups
Frequency of treatment:	Daily
Control group and treatment:	Yes (concurrent, dosed with 5% isopropanol at a volume of 2 ml/kg)
Duration of test:	Days 0 - 19 of gestation
Statistical methods:	None
Remarks:	The test substance, in the vehicle 5% isopropanol, was applied topically to five groups of artificially inseminated female rabbits (8 rabbits/group). The vehicle alone was applied topically to one group of 8 rabbits. Animals were treated at dose levels of 0, 10, 20, 40, 100 and 200 mg/kg/day at a dosage volume of 2 ml/kg. Animals were treated with the test substance or vehicle for four hours each day for 13 consecutive days on presumed day of gestation 6 through 18. Because of test substance-related mortality and severe topical effects, administration of the 100 and 200 mg/kg/day dosages were discontinued after the eighth and sixth daily dosages, respectively. As there was not a "no effect" level, two additional groups (8 rabbits/group) were treated with a second vehicle control and a new low dosage (2 ml/kg) of the test substance (2.0 mg/kg/day). These rabbits were not inseminated and were given the test substance or vehicle alone for 13 consecutive days. Test substance solutions were prepared on a weekly basis, or as needed. Animals were observed daily during the dosage and postdosage periods for signs of toxicity, skin irritation, abortion (inseminated rabbits),

death, body weight and feed consumption. Rabbits that died during the test were examined for pregnancy, if appropriate, and cause of death. On gestation day 19, all surviving females were sacrificed and a complete gross necropsy was performed, including examination of the brain. The uterus was examined for pregnancy, number of implantations and corpora lutea, live and dead fetuses, and early and late resorptions. The noninseminated rabbits similarly were sacrificed and necropsied approximately 24 hours after the 13th daily dosage was administered. This study was conducted to determine dosages of the test substance to be administered topically to rabbits in a subsequent teratology study.

Results

Maternal toxicity NOEL:	50 mg/kg/day
Developmental toxicity NOEL:	150 mg/kg/day
Actual dose received:	0, 2, 10, 20, 40, 100 and 200 mg/kg/day
Maternal data:	Three of eight rabbits each in the 100 and 200 mg/kg/day dosages died or were moribund sacrificed. Because of test substance related mortality, administration of these dosages was discontinued after the eighth and sixth daily dosages, respectively. Clinical observations noted in animals dosed at 40, 100 and 200 mg/kg/day, and considered to be effects from the test substance, included uncoordinated movement, partial paralysis, red exudate of vaginal origin present in the cage pan, green matted fur, ataxia and and/or alopecia. All skin reactions, including erythema, desquamation, atonia, fissuring, eschar and/or exfoliation demonstrated dosage-dependent onset incidence and severity. All rabbits in each of the dosage groups had a minimum of Grade 1 erythema observed at least once. No rabbit in any dosage group exhibited edema and no vehicle control rabbit had any of these signs of skin reaction present. Average body weight gain was inhibited by administration of dosages of 2.0 through 200 mg/kg/day of the test substance, as compared with the control group. The body weight effect was dosage dependent and considered to be biologically significant at dosages of 10.0 through 200 mg/kg/day. The severity of the effect ranged from slight, for 2.0 and 10.0 mg/kg/day dosage group rabbits, to marked, for 100 and 200 mg/kg/day dosage group rabbits. Reduced average daily feed consumption was noted in the 2.0 through 200 mg/kg/day dosage groups in an apparent dose-related trend. It was considered biologically

significant for rabbits in the 400 through 200 mg/kg/day dosage groups. Pregnancy occurred in 6 or 7 of the 8 rabbits in each dosage group. Upon completion of Caesarean-sectioning, a complete gross necropsy was performed on the does.

Fetal data: Litter parameters:
An increase incidence of resorptions was observed in maternally toxic dosages of 40, 100 and 200 mg/kg/day. In the 100 and 200 mg/kg/day dosage groups, an associated decrease in average litter size (live fetuses) was observed.
Fetal evaluations:
All fetuses were alive at maternal Caesarean-sectioning.

Statistical results: None

Remarks:

Conclusions

Remarks: Dosages of 0.0, 2.0, 10.0 and 20.0 mg/kg/day of the test substance were recommended for use in the definitive rabbit teratology study (author of the report). The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 2B

Remarks: Reliable with restrictions; basic data given, comparable to guidelines/standards.

References

Hoberman, A. M. and M. S. Christian. 1984. Initial submission: Pilot Study for Percutaneous Teratology of 1-Hexadecanaminium & 5% Isopropanol in Rabbits with Attachments and Cover Letter Dated 07/279/2. EPA document number 88-920004922. Argus Research Laboratories, Inc., Horsham, PA, U. S.

Other

Last changed: July 25, 2000

Order number for sorting: 60

Remarks:

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Test Substance

Identity:	1-Hexadecanaminium (CAS RN 693-33-4; Ammonium, (carboxymethyl) hexadecyldimethyl-, hydroxide, inner salt)
Purity:	30.4%
Remarks:	

Method

Method/guideline followed:	Not stated
GLP:	Yes
Year:	1984
Species:	Rat
Strain:	COBS® CD
Route of administration:	Oral gavage
Doses/concentration levels:	0, 50, 150 and 250 mg/kg/day
Sex:	Female
Exposure period:	Days 6 - 15 of gestation
Frequency of treatment:	7 days/week
Control group and treatment:	Yes (concurrent, dosed with ethanol in deionized water at a volume of 5 ml/kg)
Duration of test:	Days 0 - 20 of gestation
Statistical methods:	Fetal sex ratios and the proportions of liters with malformations were compared using the Chi-square test and/or Fisher's Exact probability test. The proportions of resorbed and dead fetuses and postimplantation losses were compared by the Mann-Whitney U-test. The mean number of corpora lutea, total implantations, live fetuses and mean fetal body weights were compared by ANOVA (one-way) Bartlett's test for homogeneity of Variances and the appropriate t-test.
Remarks:	Dosage calculations were based on a 100% active component. Since the test substance was received with a 30.4% active moiety in 10% ethanol, a correction factor of 3.2895 was utilized to achieve the proper amount of active ingredient. The control group received ethanol in deionized water at a volume of 5 ml/kg. The amount of ethanol the control group received was equal to the amount given to the 250 mg/kg/day group. The stock solution was prepared daily. Dose volume was 5 ml/kg body weight, adjusted for body weight on days of gestation 6, 9 and 12. Animals were observed twice daily for signs of toxicity. Body weights were recorded on day 0, 6, 9, 12, 16 and 20 of gestation. Food consumption intervals were identical to the body weight intervals. On gestation day 20, all

surviving females were sacrificed by carbon dioxide inhalation. The uterus was exposed and the lumber and location of viable and nonviable fetuses, early and late resorptions and the number of total implantations and corpora lutea were recorded. The uterus was then excised and the fetuses were removed. Live fetuses were individually weighed, sexed, tagged and examined for external malformations or developmental variations. Approximately one half of the fetuses for each litter were fixed in Bouin's solution to examine the viscera and brain by Wilson's sectioning technique. The remaining one-half of the fetuses were processed (alizarin red staining) and examined for skeletal abnormalities.

Results

Maternal toxicity NOEL:	Not stated
Developmental toxicity NOEL:	Not stated
Actual dose received:	0, 50, 150 and 250 mg/kg/day
Maternal data:	No deaths occurred in any dams in the control or treated groups. Clinical observations noted in animals dosed at 250 mg/kg/day included stained and matted fur (noted primarily on the limbs, neck, ventral thorax and facial area), excessive salivation, respiratory rales, diarrhea, decreased activity, hypothermia, lacrimation, labored breathing and wheezing. Similar observations were evident at 150 mg/kg/day group, stained and mattered fur and respiratory rales were the predominant observations. A dose-related trend of maternal body weight inhibition was noted during both the overall gestation (days 0 - 20) and treatment (days 6 - 15) periods at all dose levels. Weight loss was observed during the first treatment interval (days 6 - 9) at 150 and 250 mg/kg/day. Reduced food intake was also noted among all treated groups during the treatment period in an apparent dose-related trend. In addition, consumption was inhibited at 250 mg/kg/day during the overall gestation interval but mean values of the 50 and 150 mg/kg/day groups were comparable to controls. Necropsy revealed no treatment-related differences among the groups.
Fetal data:	<u>Litter parameters:</u> No meaningful differences among the control and treated groups were evident with respect to the number of corpora lutea, total implantations, postimplantation loss, viable fetuses and fetal body weights.

Fetal evaluations:
The incidence of fetal malformation in the treated groups was neither statistically significant nor meaningfully different from that of the controls. With respect to developmental variations, reduced or absent ossification of the skull, sternebrae #5 and/or #6 and other sternebrae occurred more frequently at the 250 mg/kg/day group. This reduced ossification of the sternebrae #5 and #6 was deemed biologically significant as it was commonly observed in conjunction with reduced maternal body weight. No further trends in developmental variations were noted.

Statistical results: Described above

Remarks:

Conclusions

Remarks: The endpoint has been adequately characterized (American Chemistry Council Fatty Nitrogen Derivatives Panel, Amides Task Group).

Data Quality

Reliability (Klimisch): 1B

Remarks: Reliable without restriction; comparable to guideline study.

References

Arnold, K. S., J. L. Schardein and M. Blair. Oral Teratology Study of 1-Hexadecanaminium in Rats. 1985. International Research and Development Corporation, U. S.

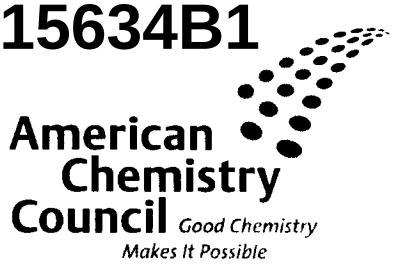
Other

Last changed: July 25, 2000

Order number for sorting: 61

Remarks:

201-15634B1



October 8, 2004

Mr. Michael Leavitt
Administrator
U.S. Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116

Attn: **Chemical Right-to-Know Program-Consortium #**

Dear Administrator Leavitt:

It is my pleasure to submit the revised Test Plan documents on behalf of the Amides Task Group of the American Chemistry Council's Fatty Nitrogen (FND) Derivatives Panel.

The FND Amides Task Group (Task Group) first submitted its FND Amides Test Plan (Test Plan) to EPA on December 20, 2001. EPA submitted comments on the Test Plan to the Task Group in a letter dated June 27, 2002.

Please direct inquiries regarding this letter to me at 703-741-5605 or Christopher_Cleet@americanchemistry.com.

Sincerely,

Christopher Cleet
Manager, FND Panel

Attachment

cc: FND Panel
Amides Task Group
Steven Russell, ACC